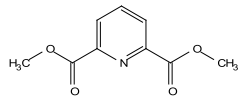
Capítulo VIII

Anexos

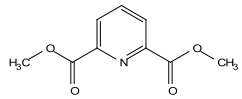
Espectros de RMN, Masas e Infrarrojo de los Precursores y Ligandos

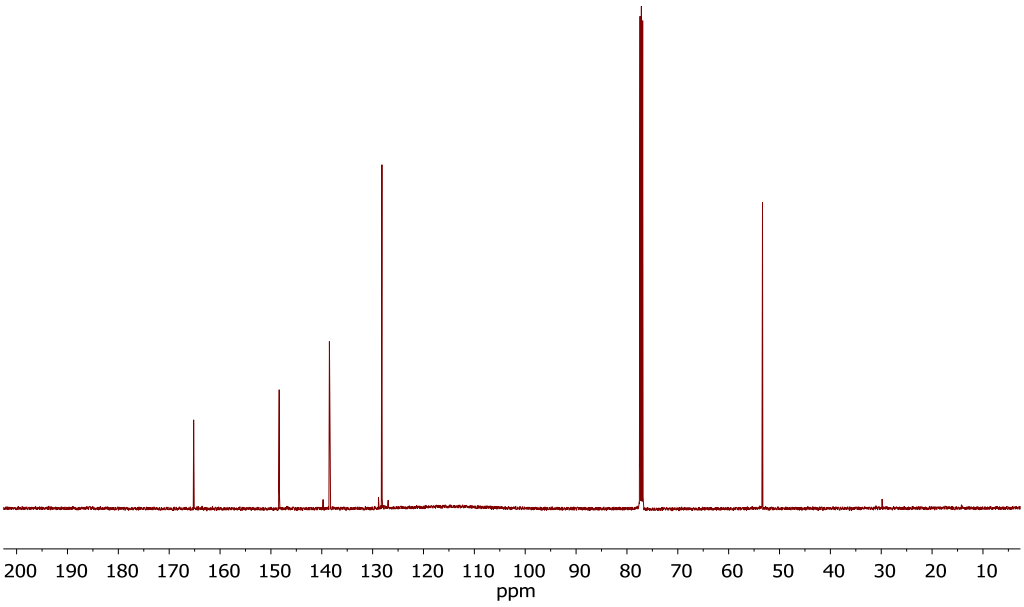
Dimetilpiridina-2,6-dicarboxilato (**1**)

^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)

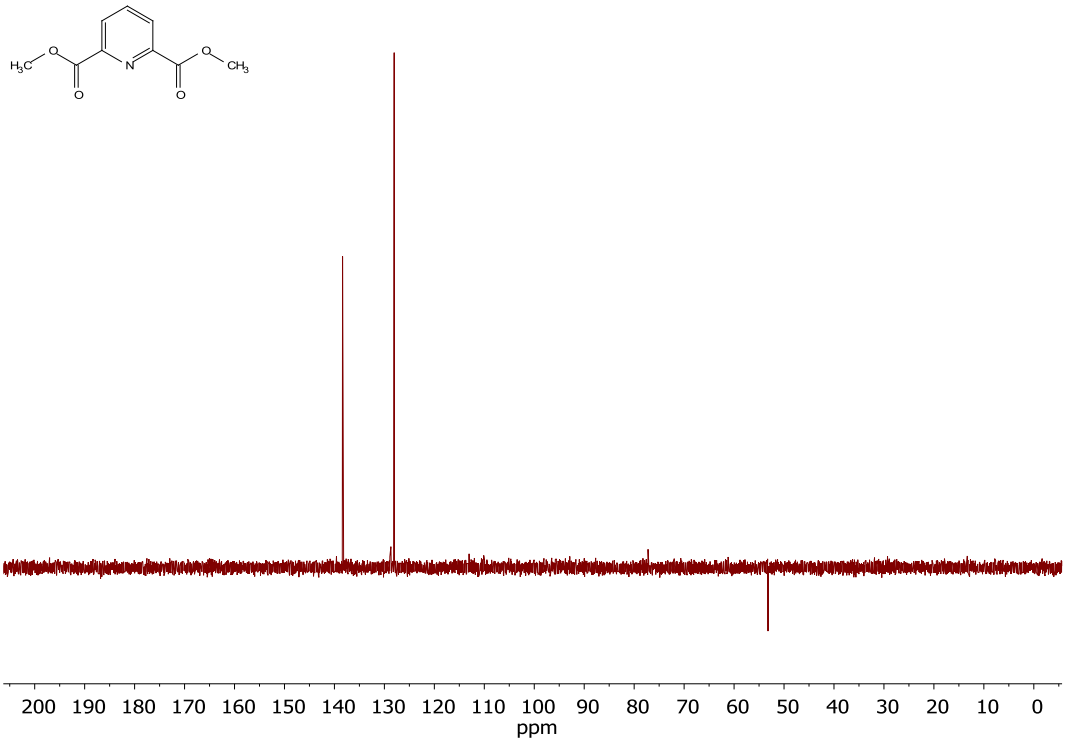


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

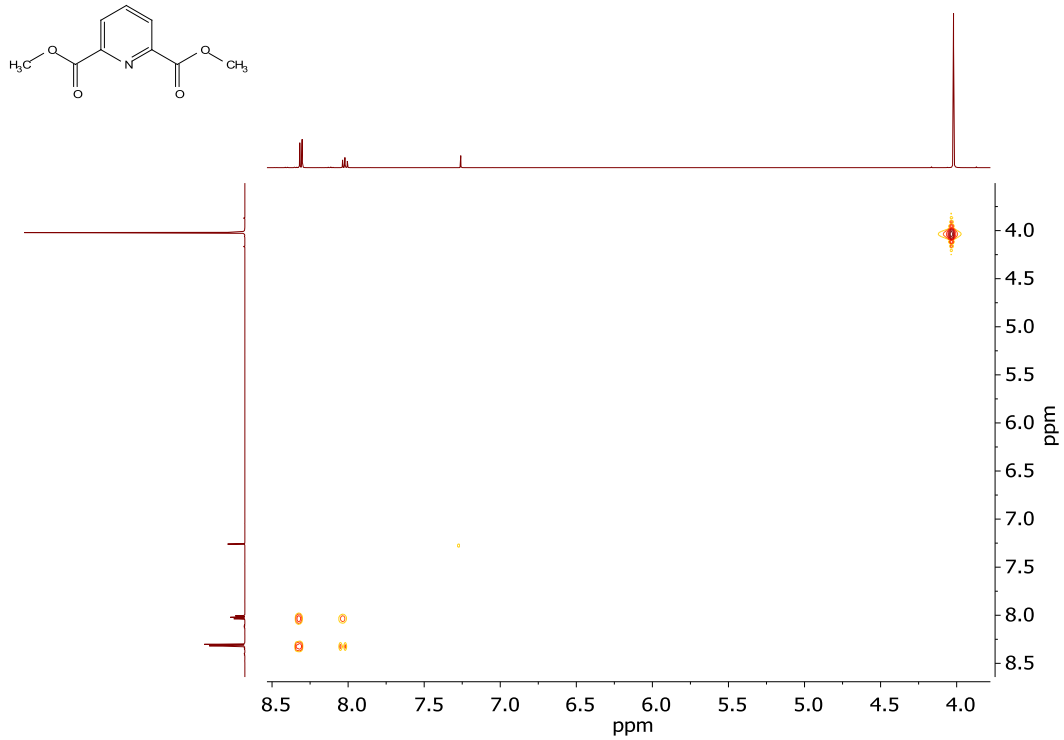




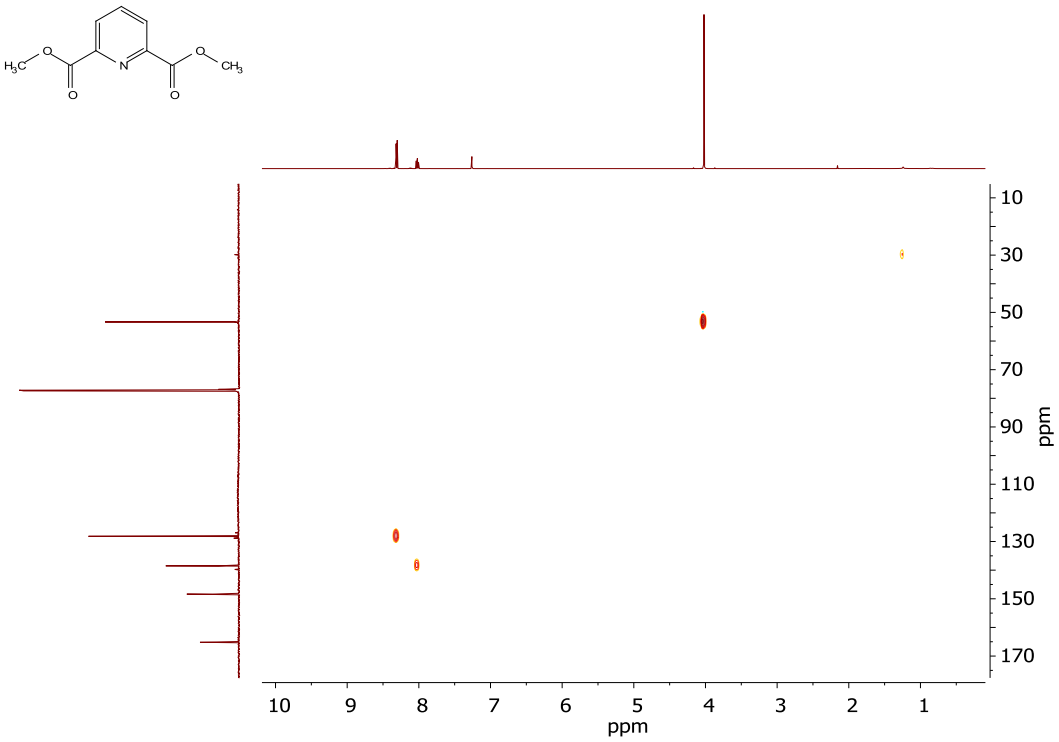
DEPT-RMN ($CDCl_3$) (δ/ppm)



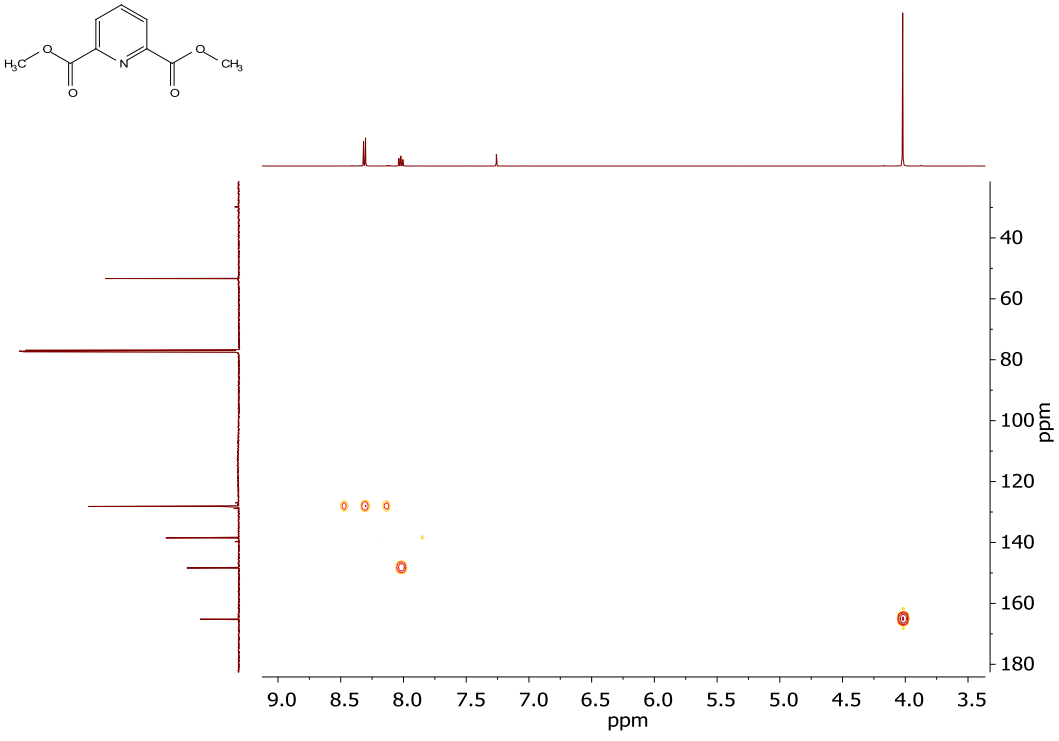
COSY-RMN ($CDCl_3$) (δ/ppm)



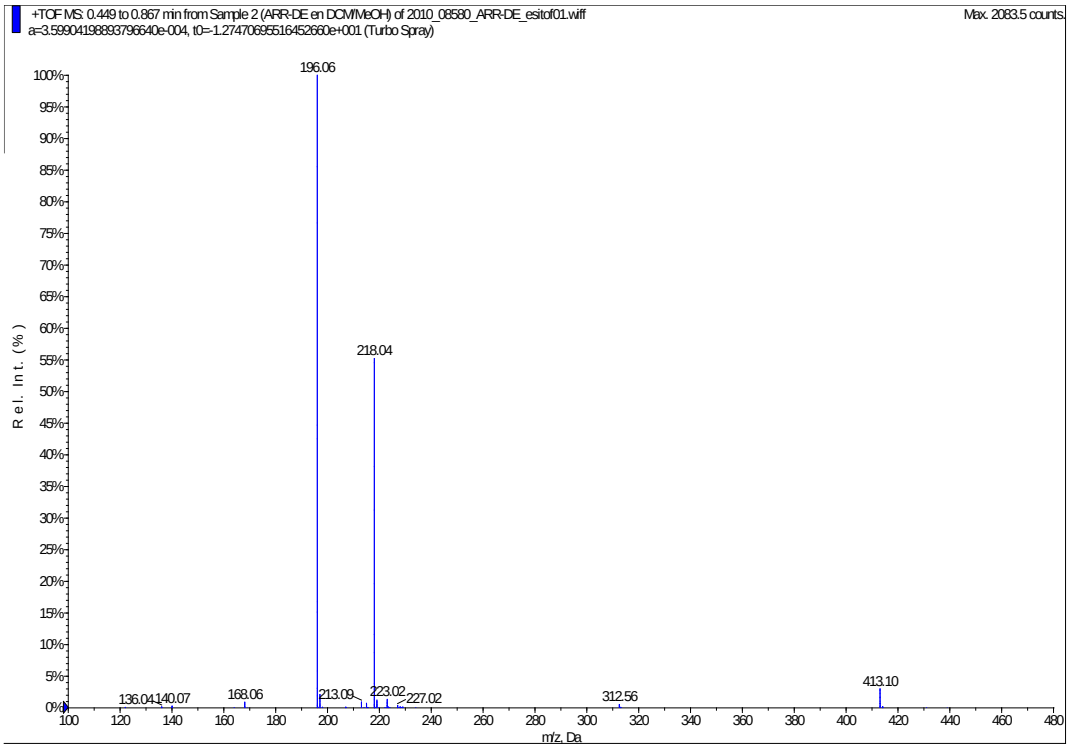
HSQC-RMN ($CDCl_3$) (δ/ppm)



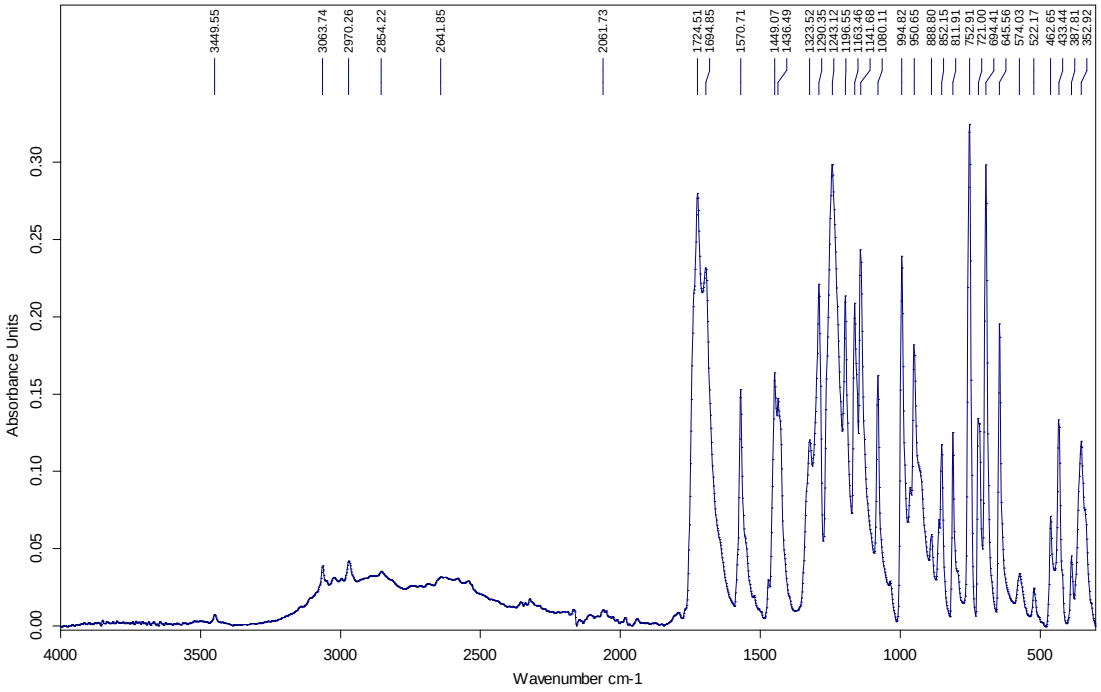
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

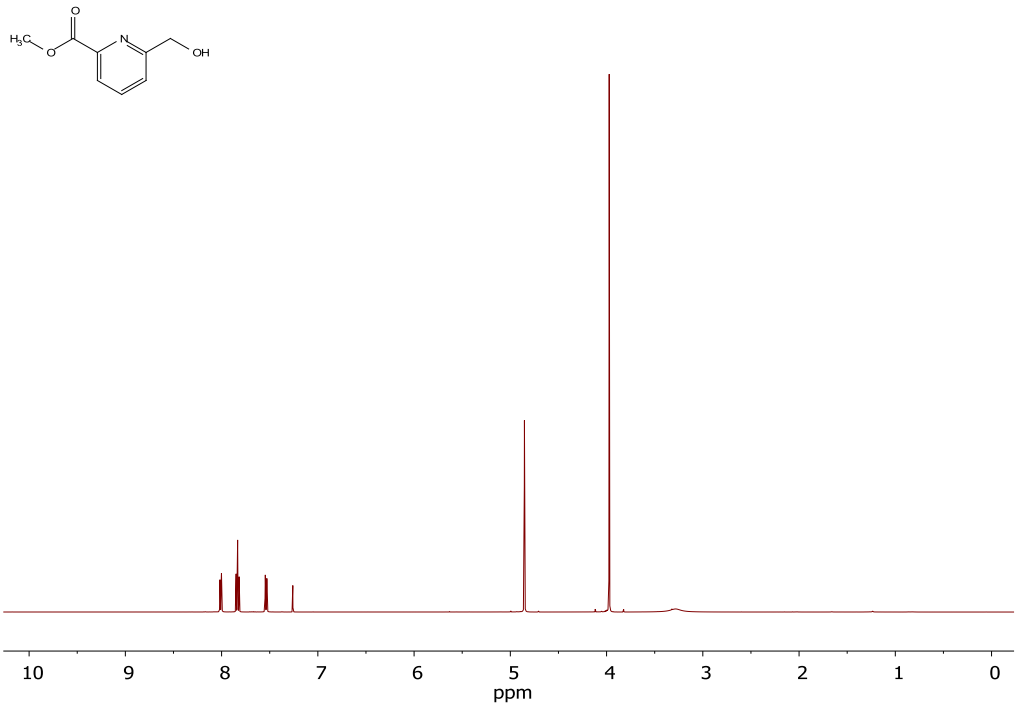


Espectro IR

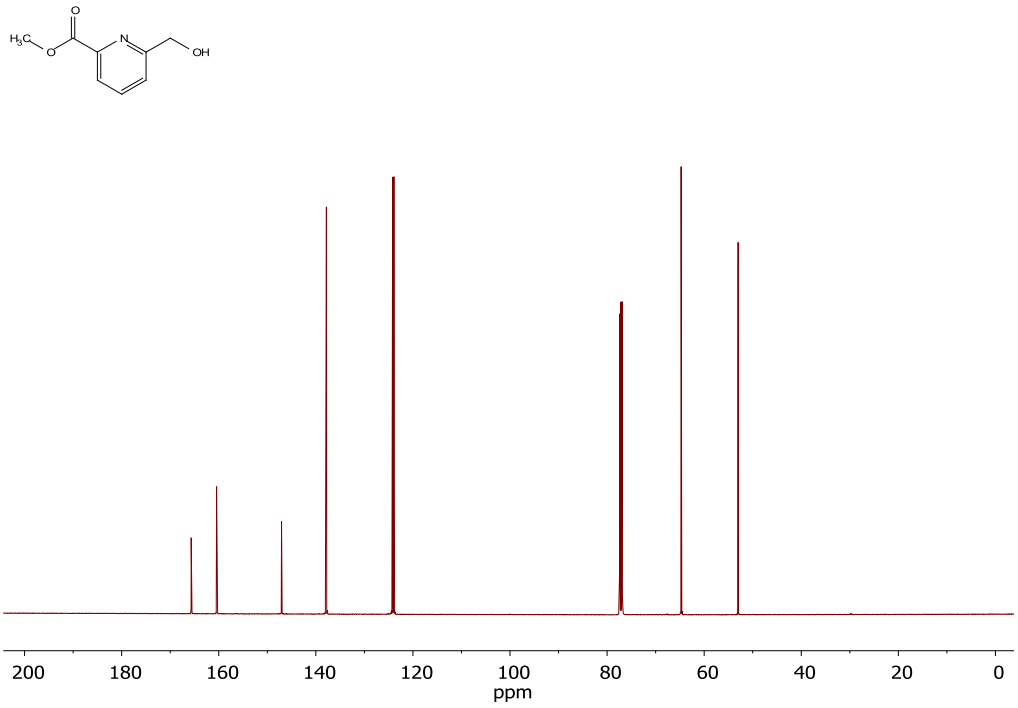


6-(Hidroximetilpiridina)-2-carboxilato de metilo (**2**)

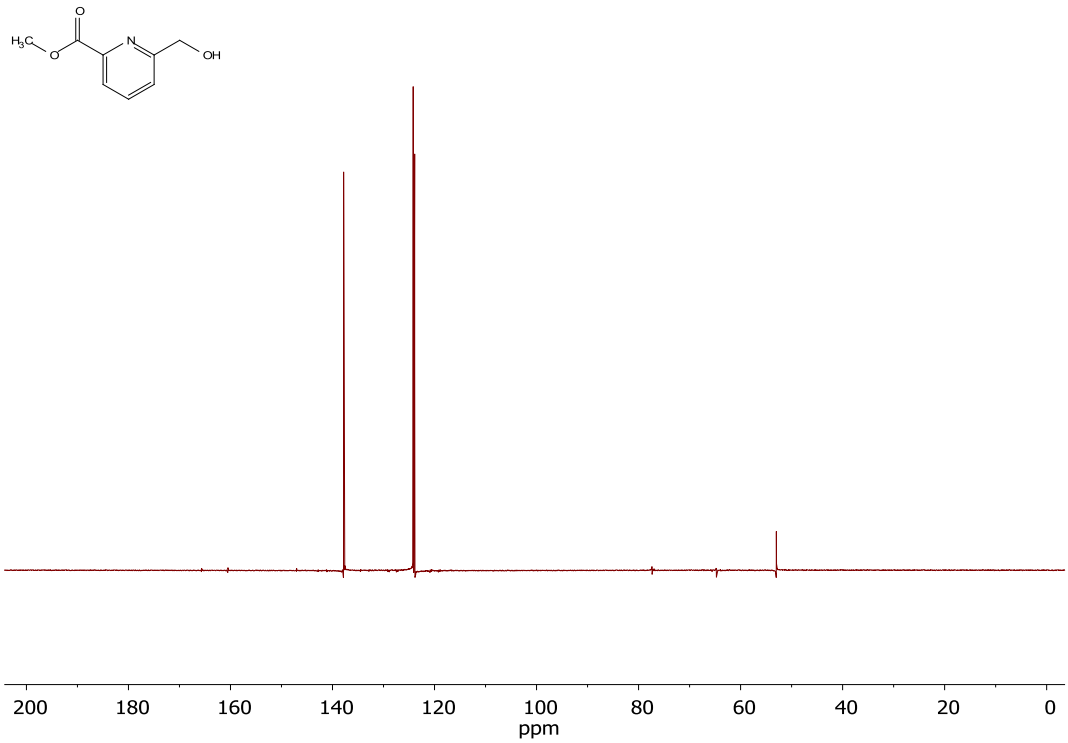
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



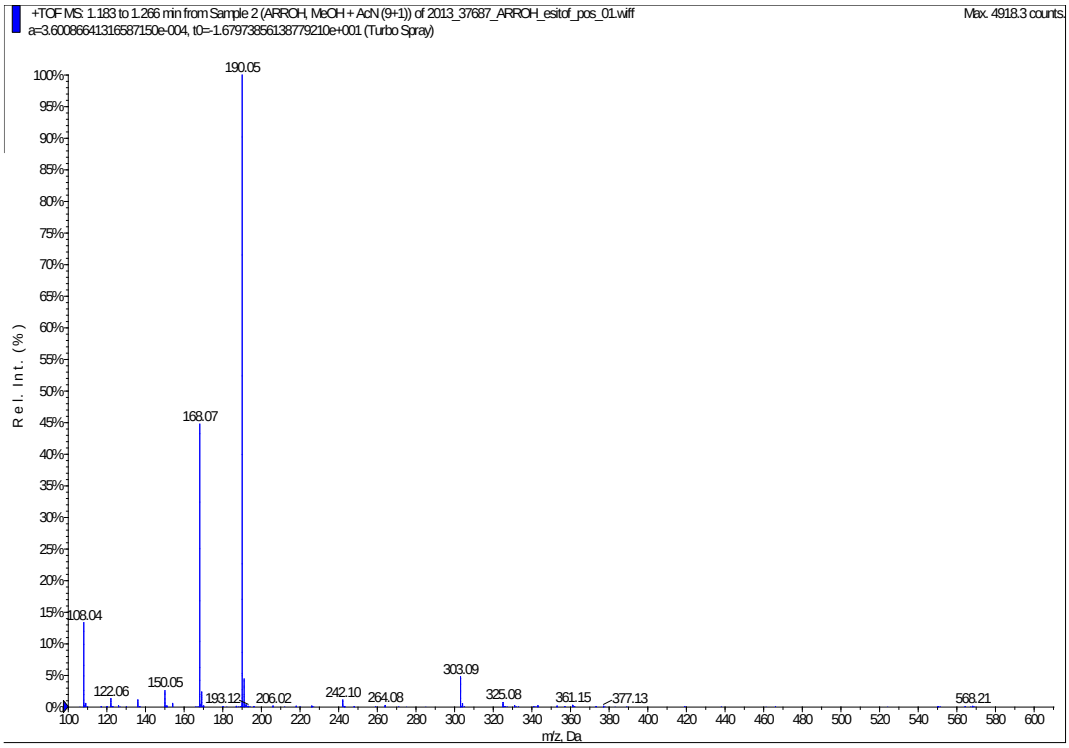
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



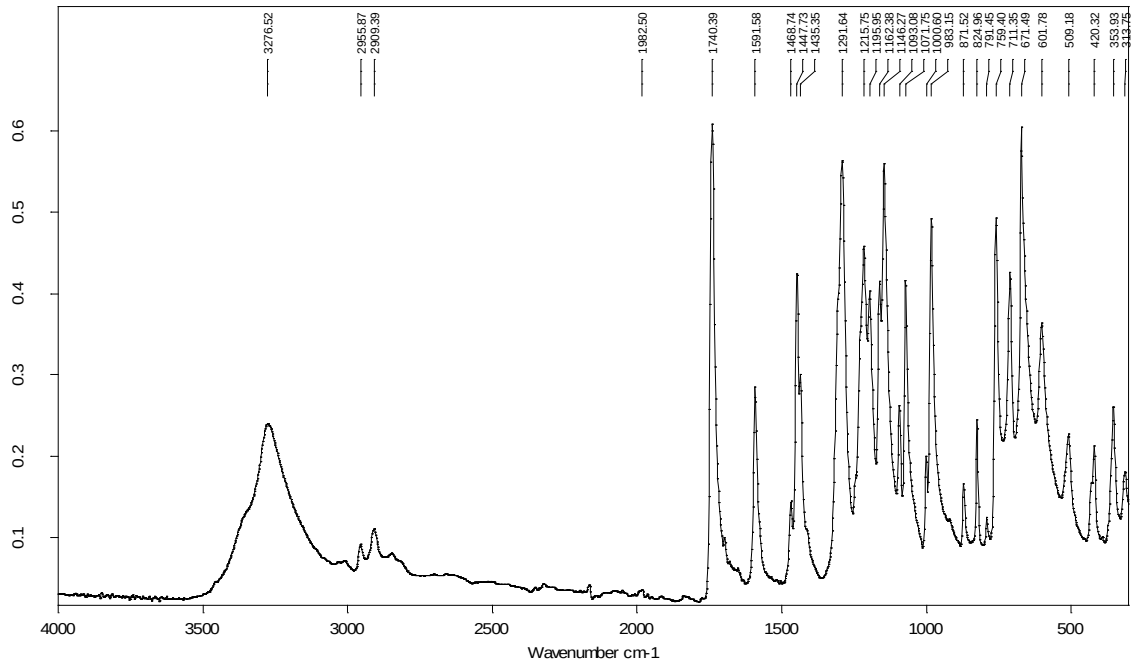
DEPT-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI^+

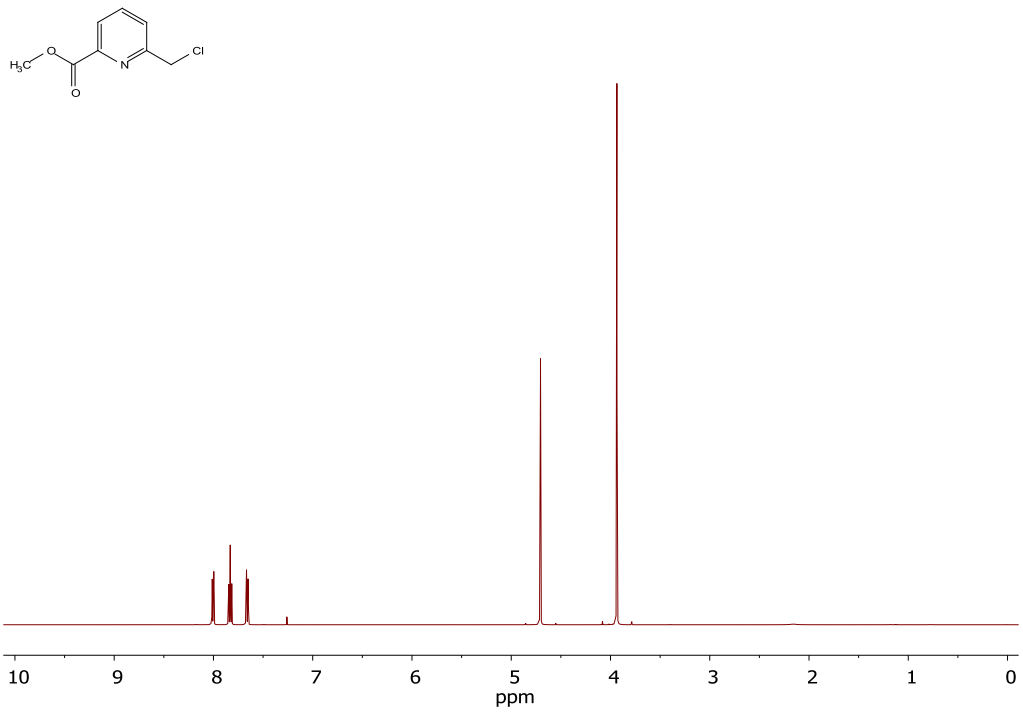


Espectro IR

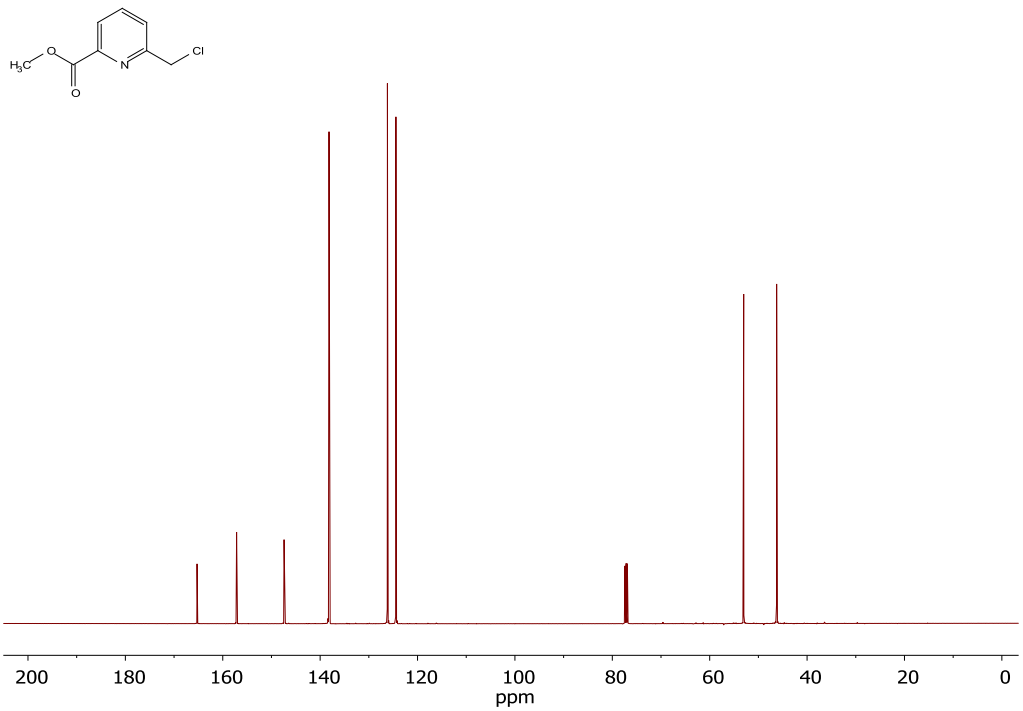

3276.52
2955.87
2909.39
1982.50
1740.39
1591.58
1468.74
1447.73
1435.35
1291.64
1215.75
1195.95
1152.38
1146.27
1093.08
1071.75
1000.60
983.15
871.52
824.96
791.45
759.40
711.35
671.49
601.78
509.18
420.32
353.93
0.1
0.2
0.3
0.4
0.5
0.6
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

6-(Clorometilpiridina)-2-carboxilato de metilo (**3**)

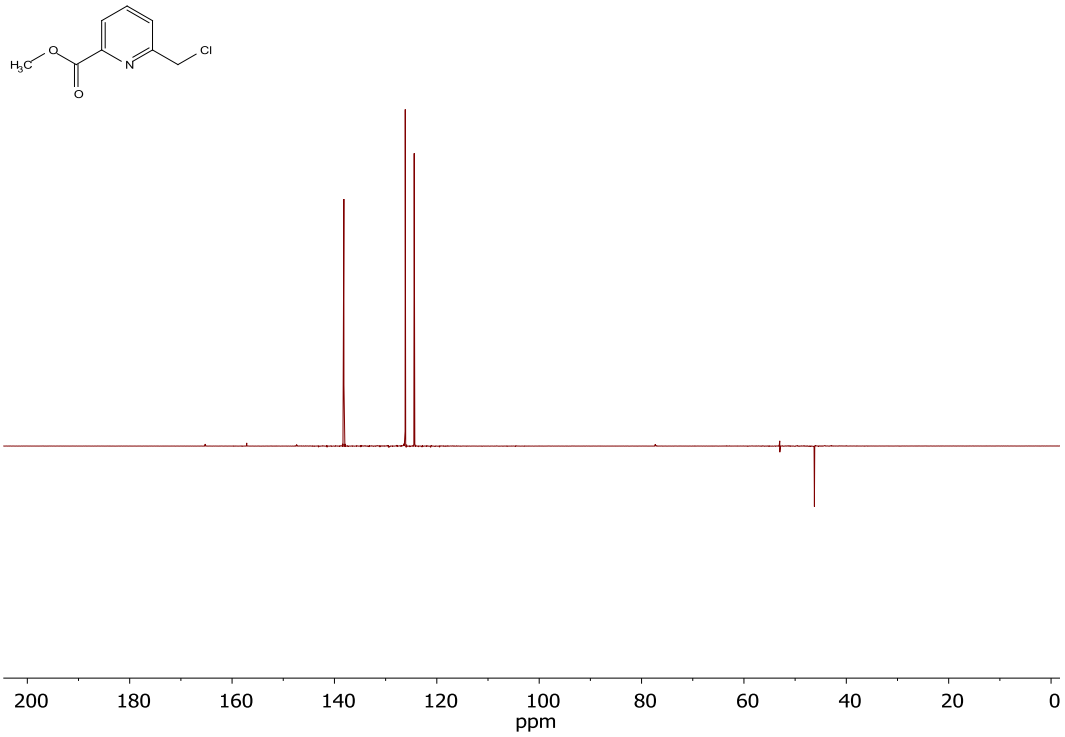
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



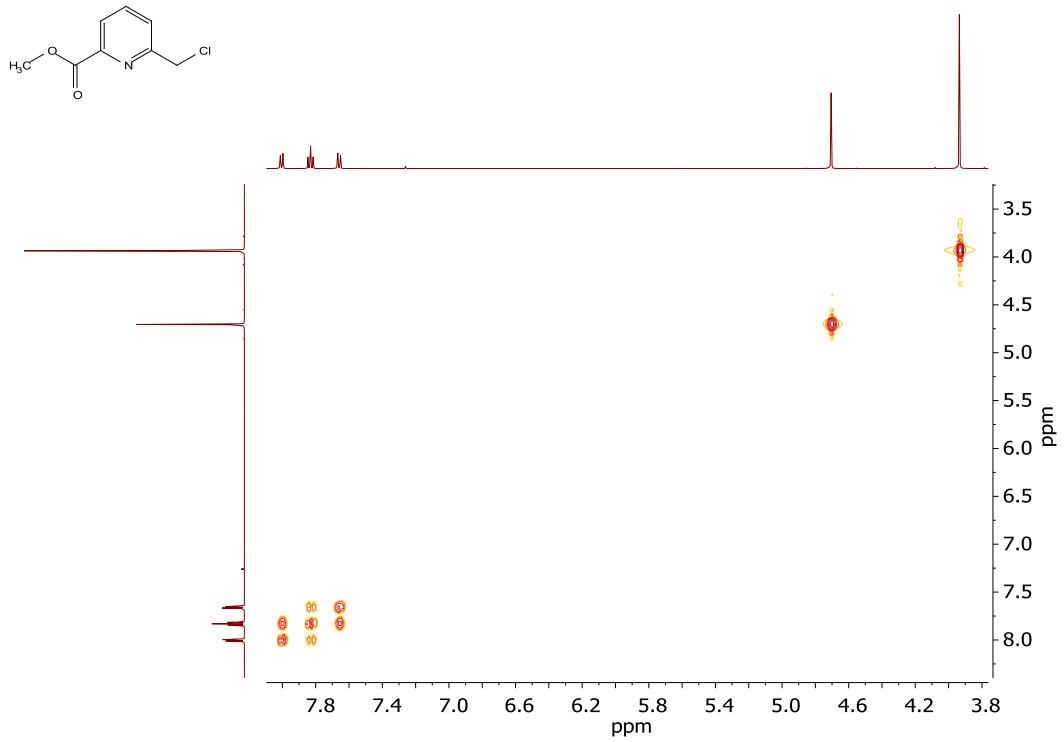
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



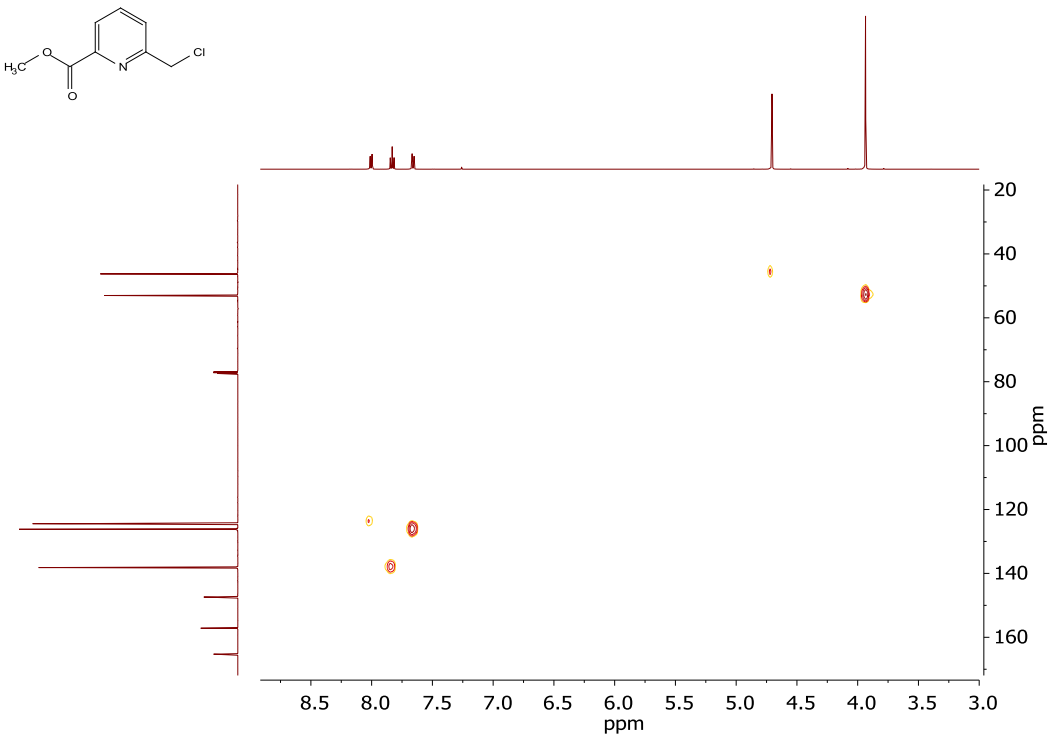
DEPT-RMN ($CDCl_3$) (δ/ppm)



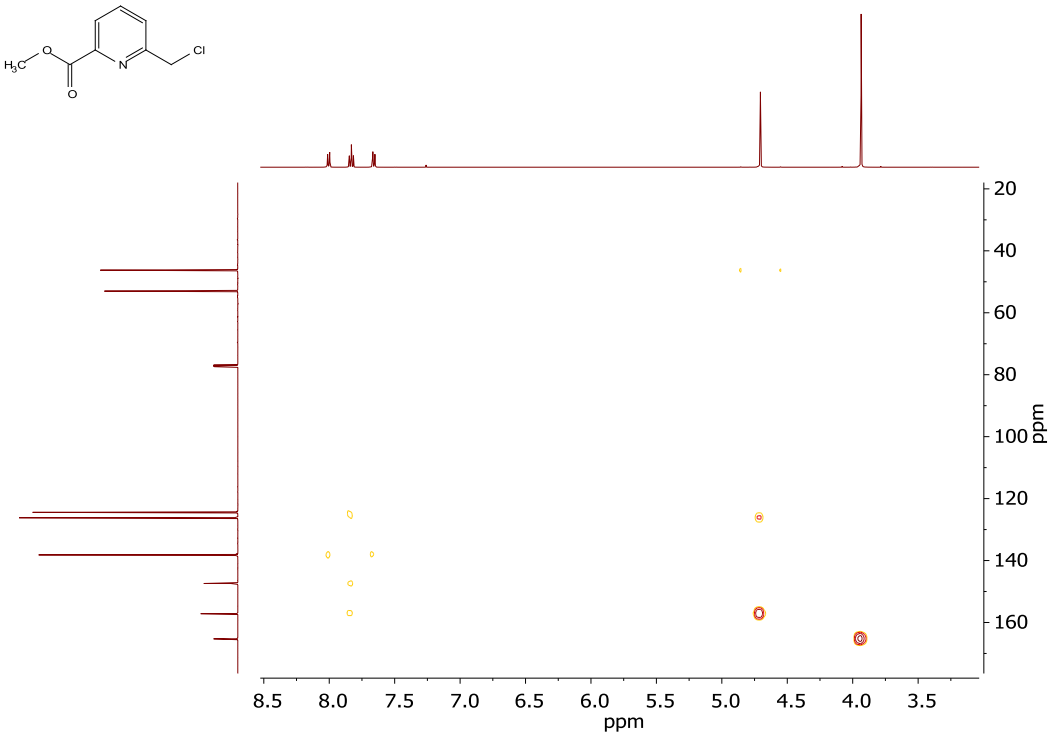
COSY-RMN ($CDCl_3$) (δ/ppm)



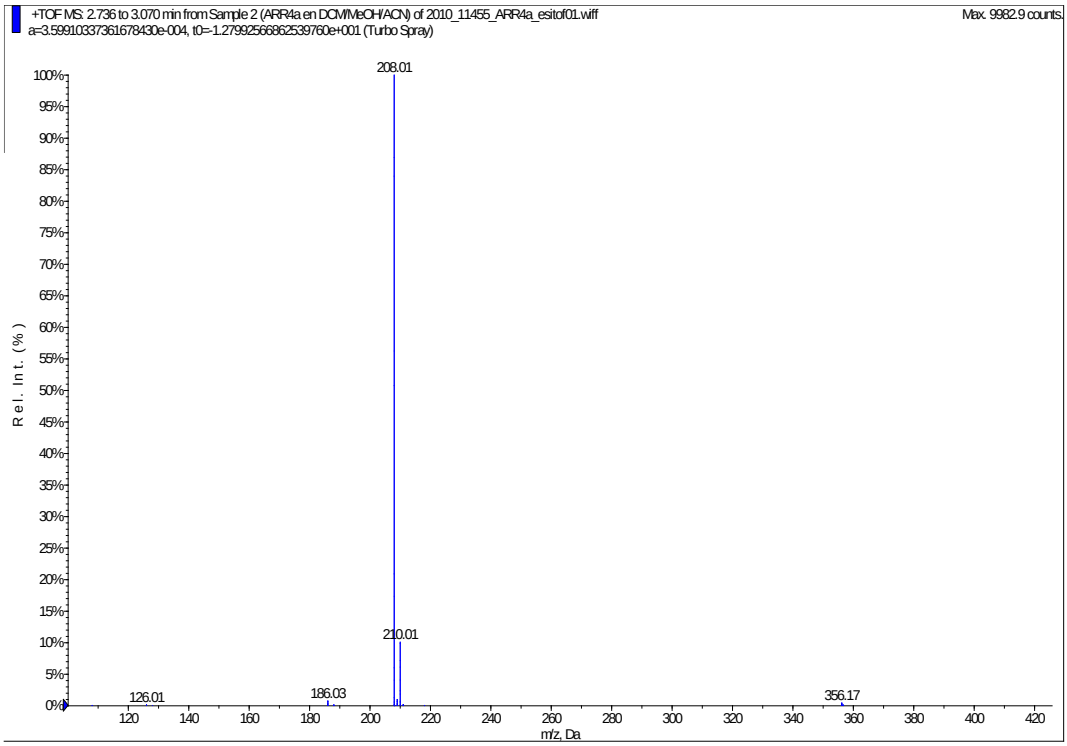
HSQC-RMN ($CDCl_3$) (δ/ppm)



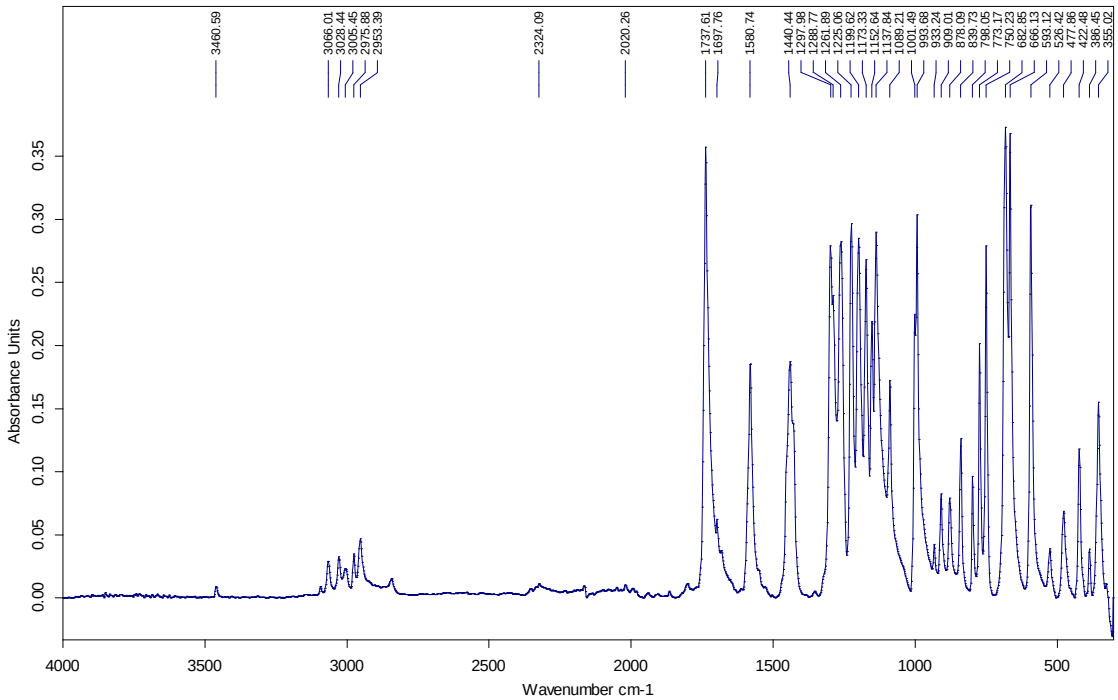
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

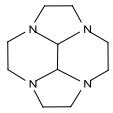


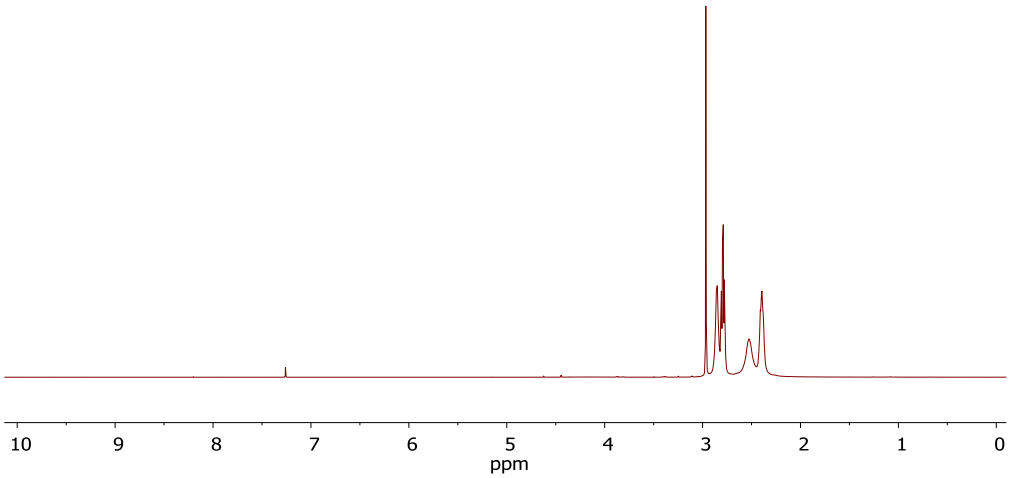
Espectro IR



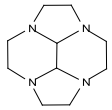
Decahidro - 2a,4a,6a,8a – tetraazaciclopenta [*fg*] acenaftileno (4)

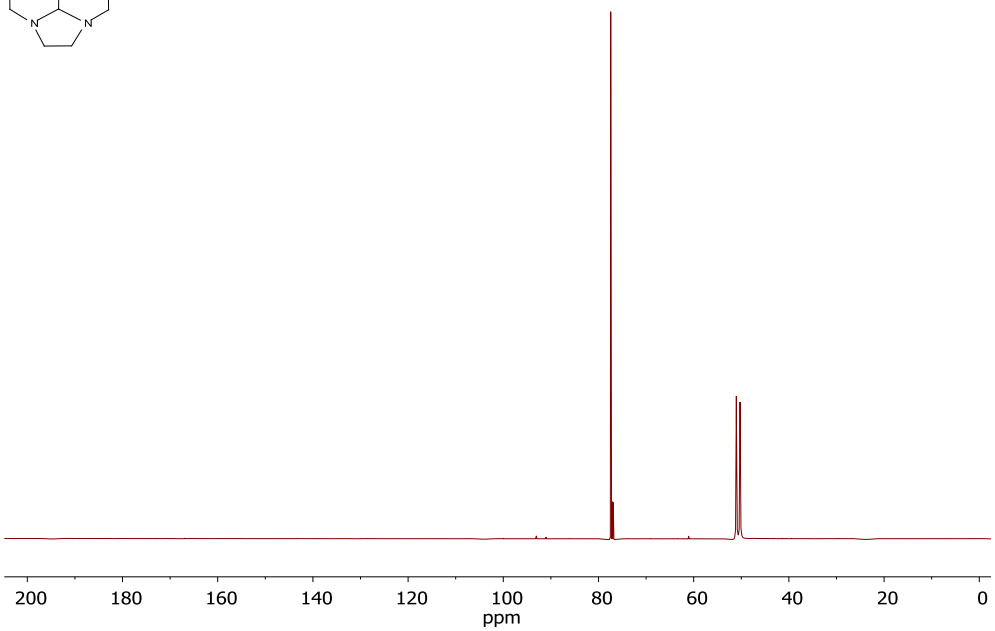
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



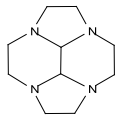


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

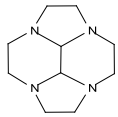




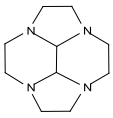
DEPT-RMN ($CDCl_3$) (δ/ppm)



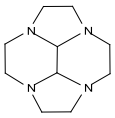
COSY-RMN ($CDCl_3$) (δ/ppm)



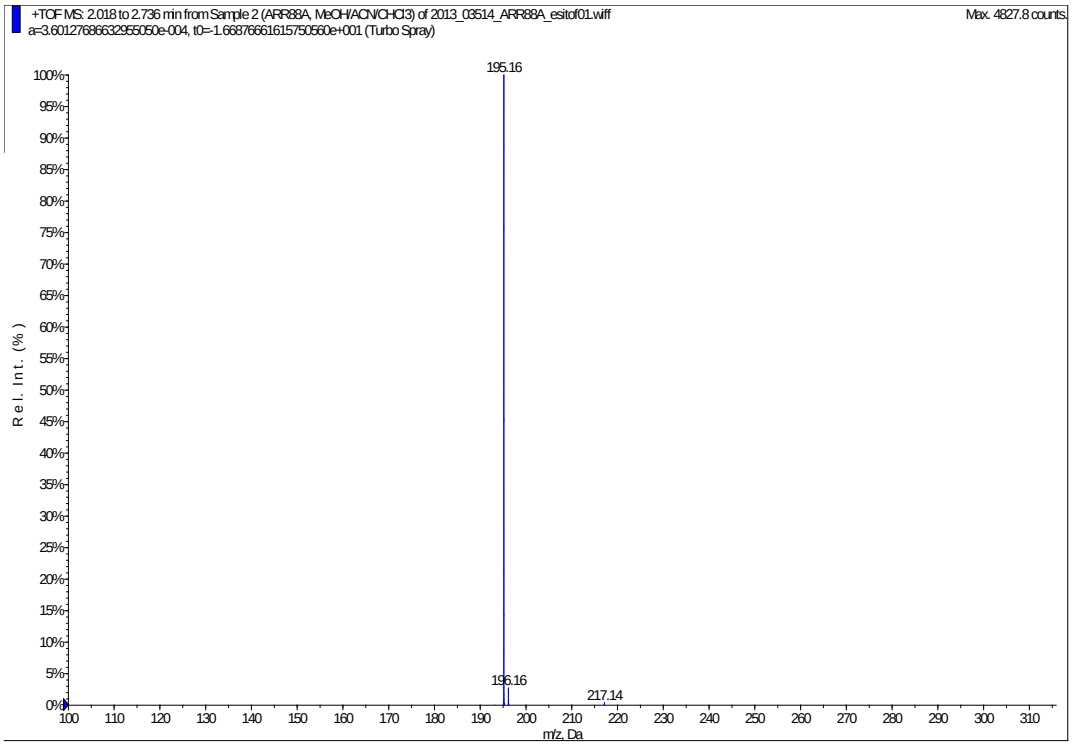
HSQC-RMN ($CDCl_3$) (δ/ppm)



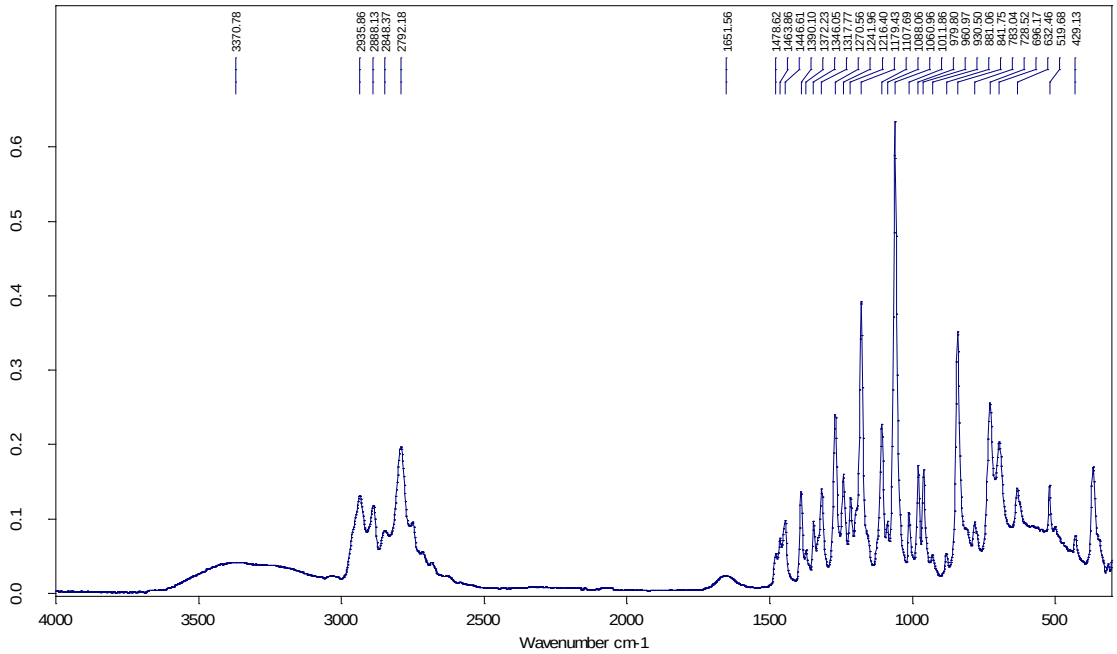
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

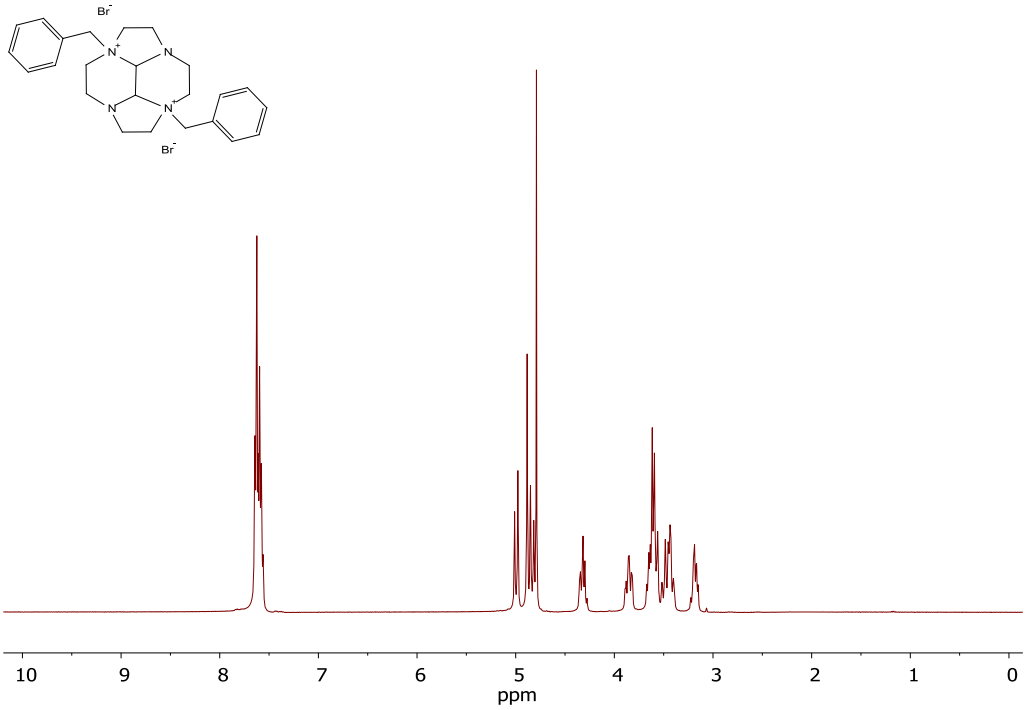


Espectro IR

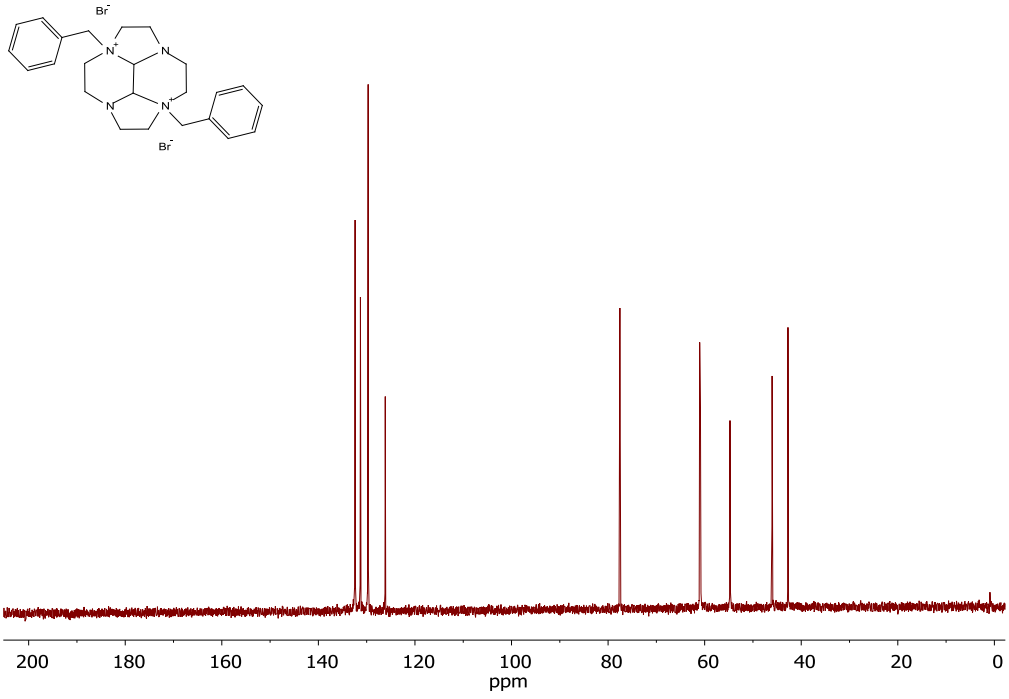


2a,6a-Dibromuro de 2a,6a – dimetildodecahidro - 2a,4a,6a,8a - tetraazaciclopenta [*fg*] acenaftileno (**5**)

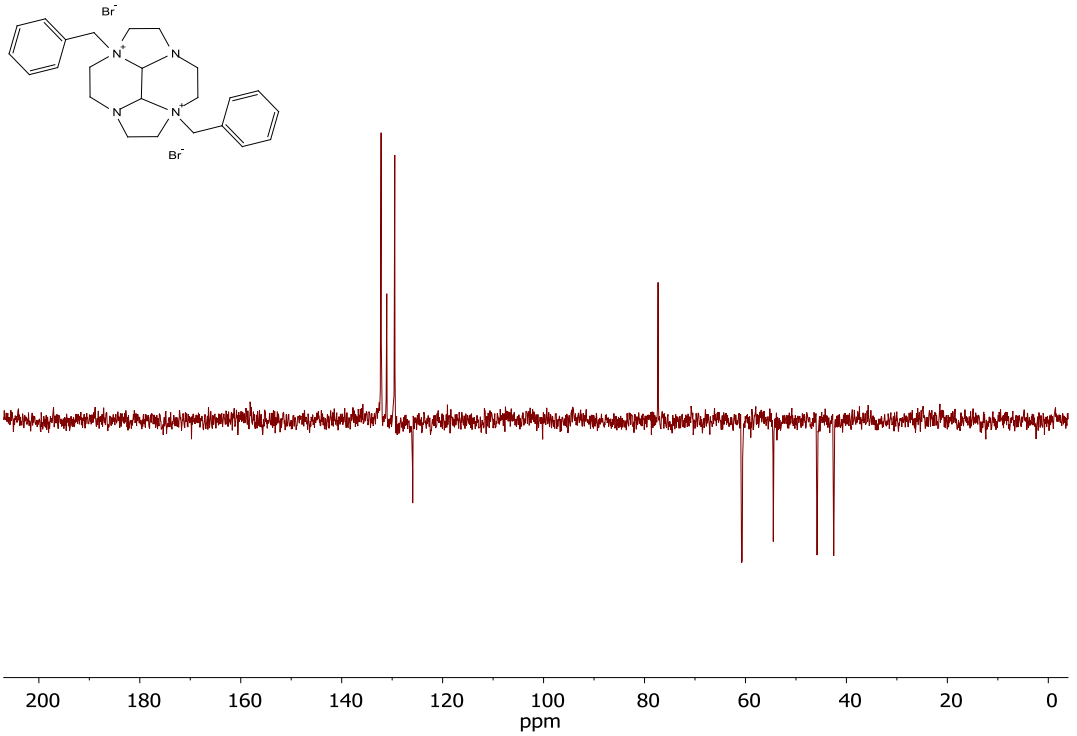
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



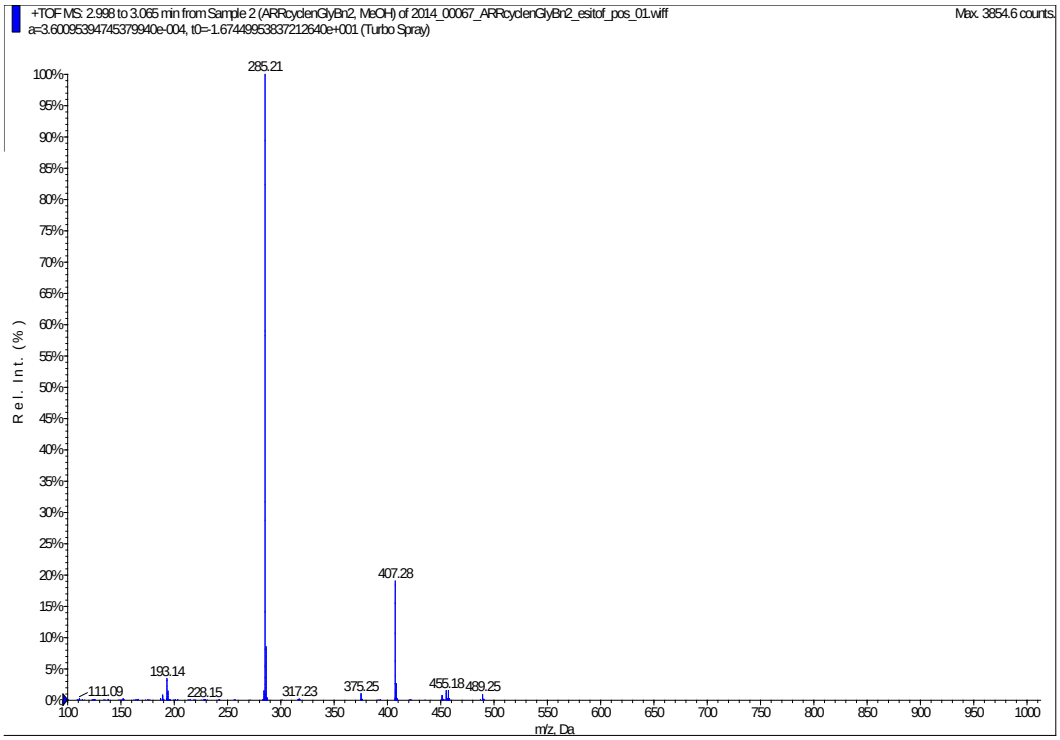
^{13}C-RMN (D_2O, 75,5 MHz) (δ/ppm)



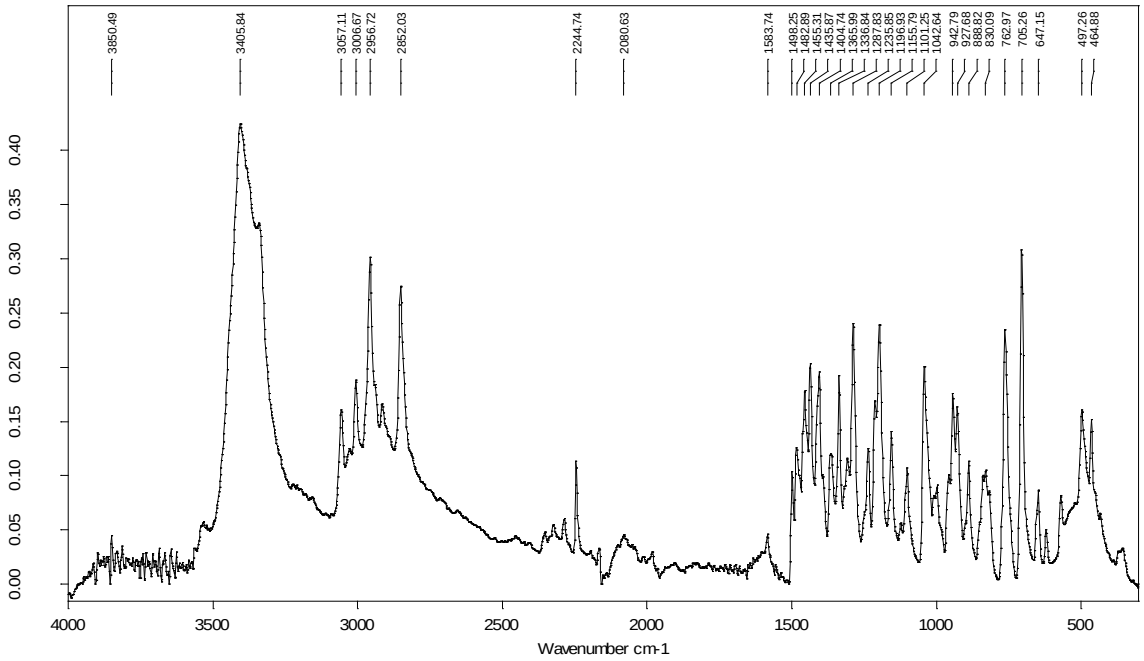
^{13}C-RMN (*J-MODE*) (D_2O) (δ/ppm)



Espectro de masas ESI$^+$

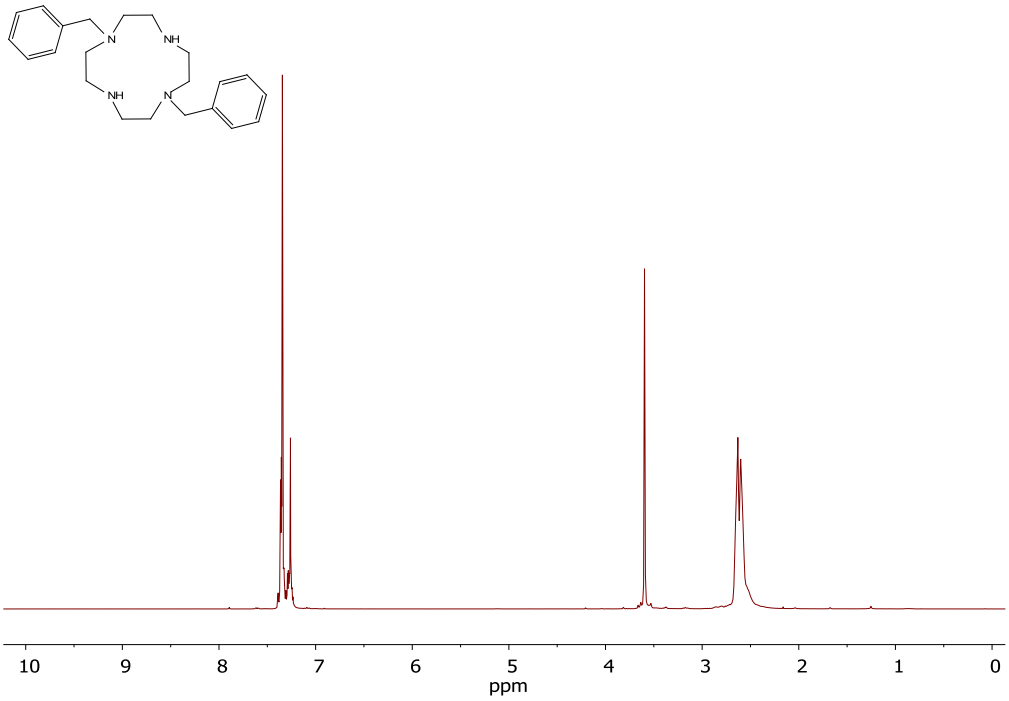


Espectro IR

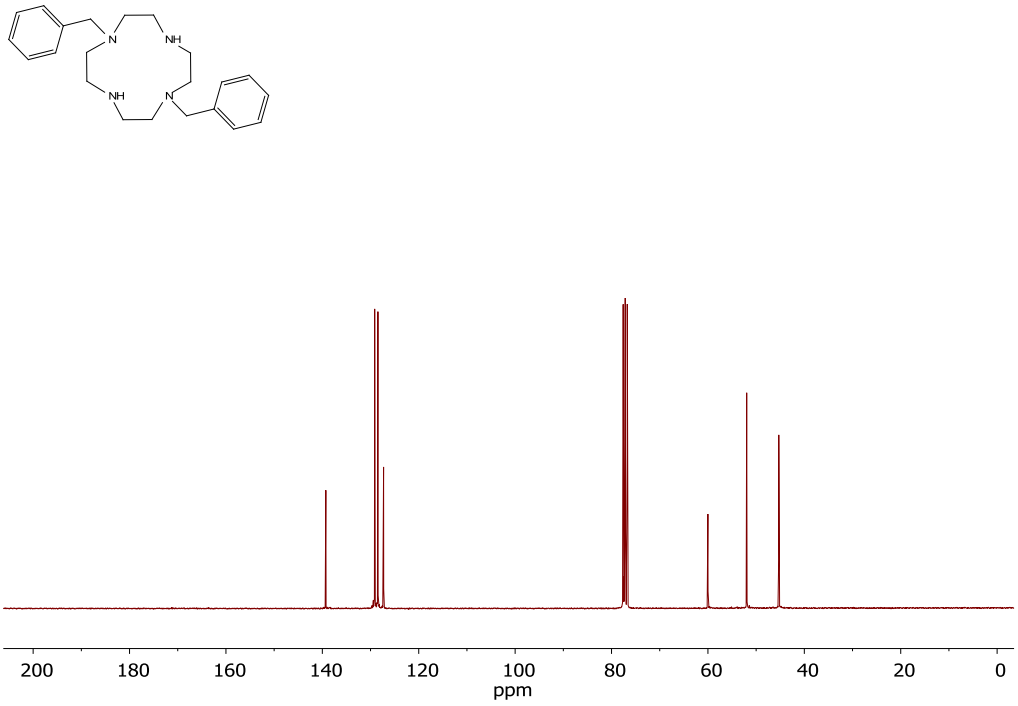

3850.49
3405.84
3057.11
3006.67
2956.72
2852.03
2244.74
2080.63
1583.74
1498.25
1482.89
1435.31
1415.87
1404.74
1365.99
1336.84
1287.83
1235.85
1196.93
1155.79
1101.25
1042.64
942.79
927.68
888.82
830.09
762.97
705.26
647.15
497.26
464.88
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

1, 7 – Dibencil – 1, 4, 7, 10 - tetraazaciclododecano – trans-ciclén dibencilo – (**6**)

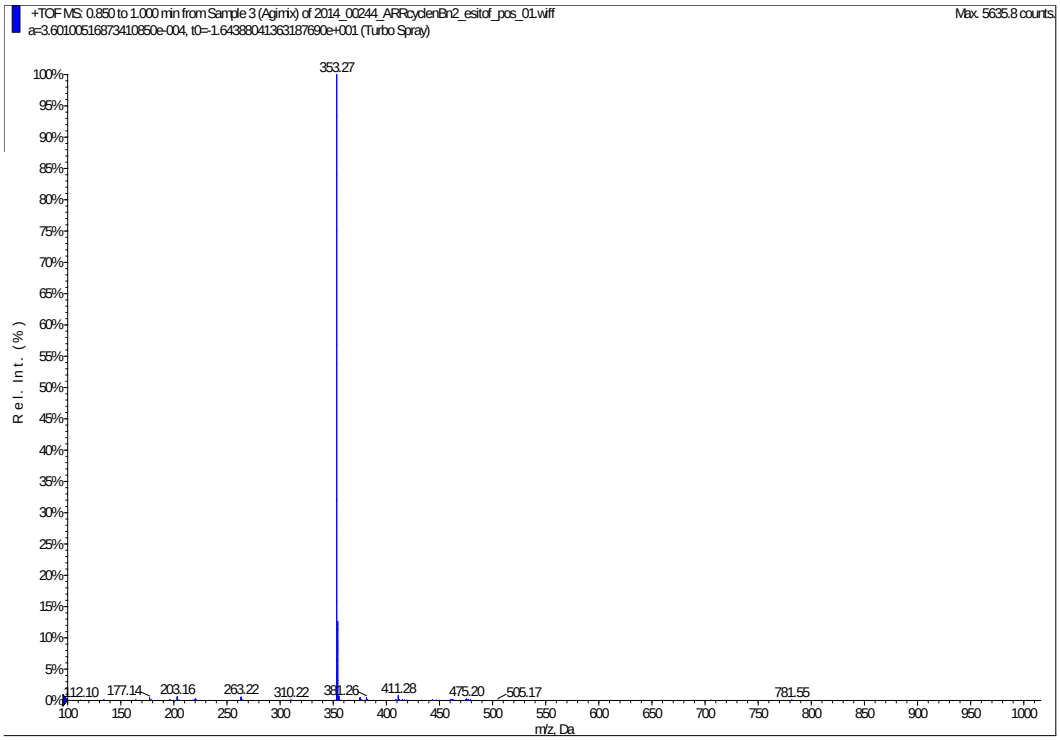
^{1}H-RMN ($CDCl_3$, 300 MHz) (δ/ppm)



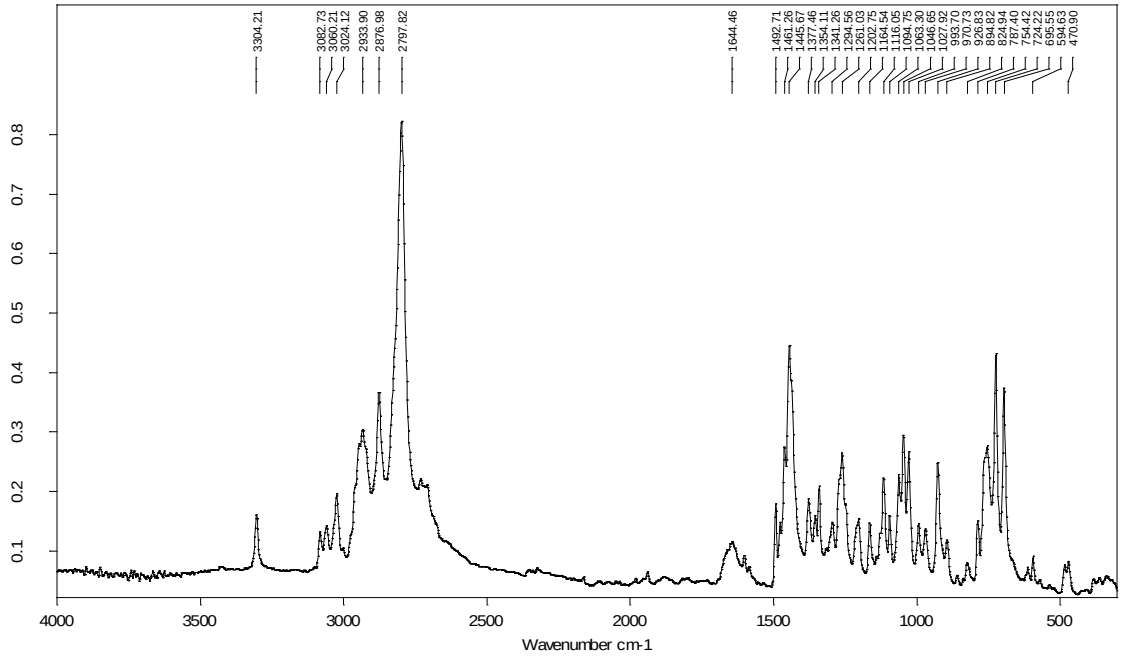
^{13}C-RMN ($CDCl_3$, 75,5 MHz) (δ/ppm)



Espectro de masas ESI+

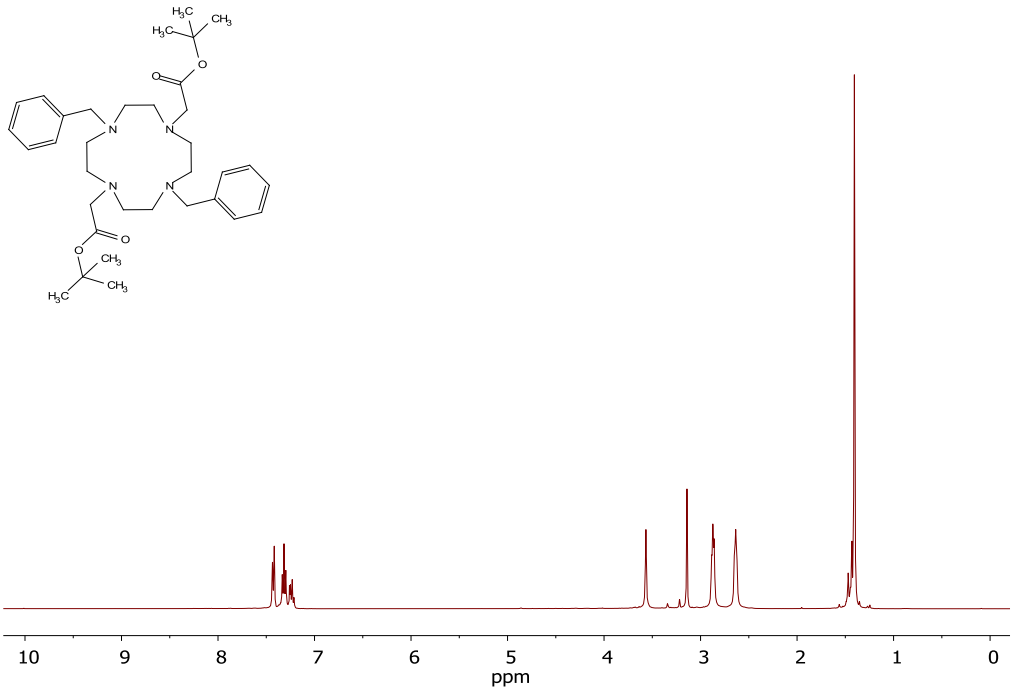


Espectro IR

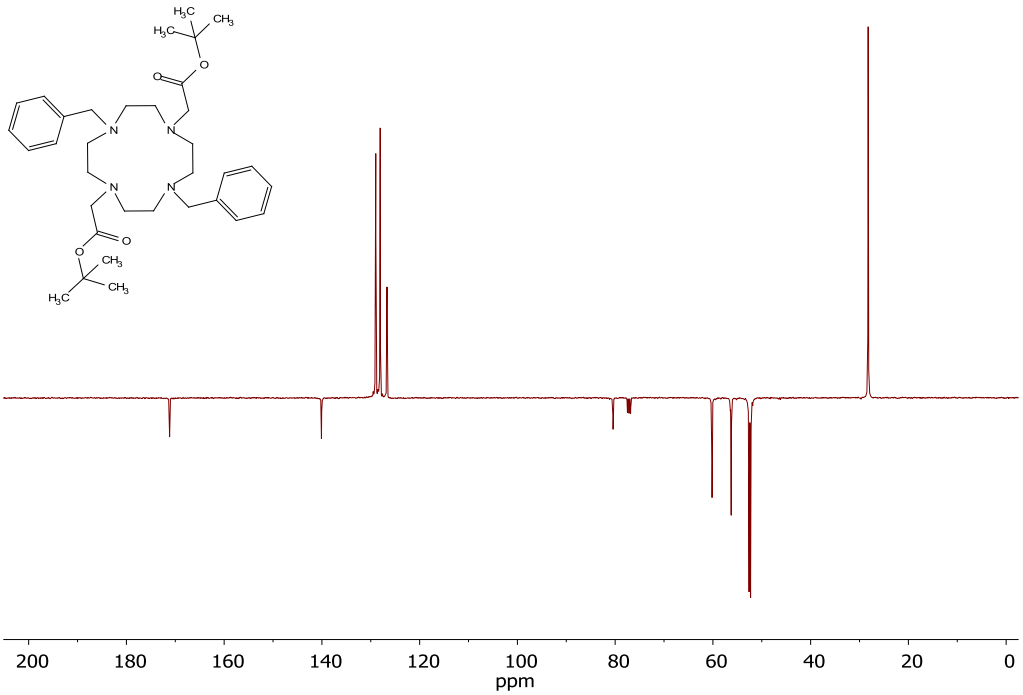


Diacetato de di – tert- butil 2, 2´ - (4, 10 – dibencil - 1, 4, 7, 10 – tetraazaciclododecano – 1, 7 – diil) (**7**)

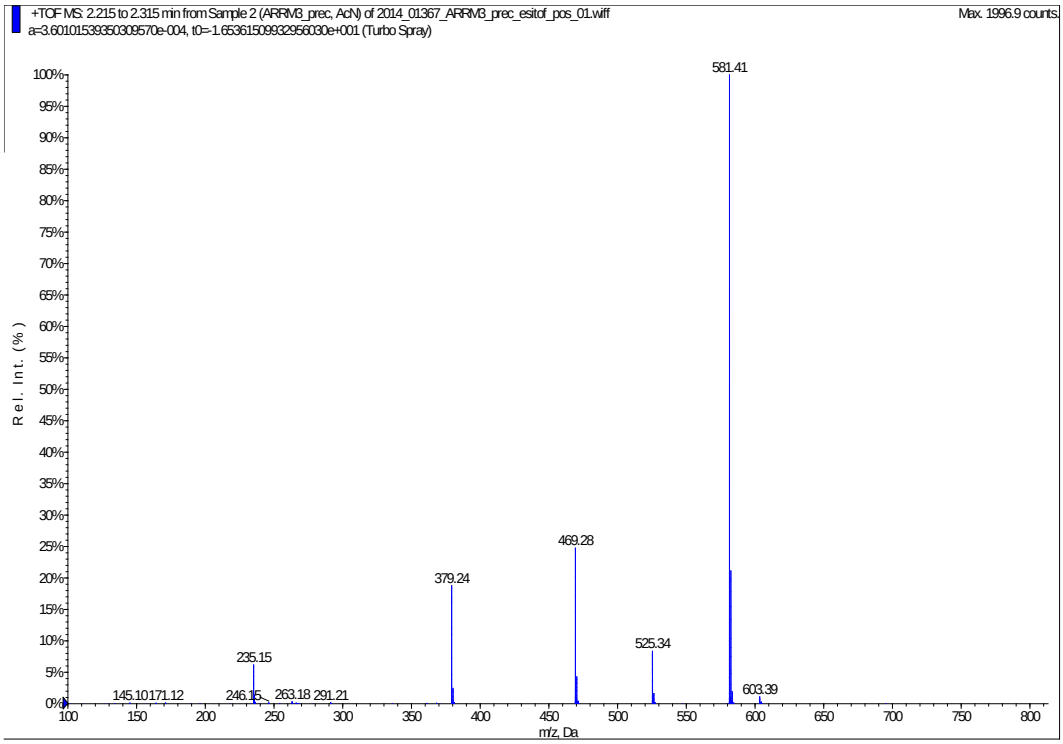
^{1}H-RMN ($CDCl_3$, 300 MHz) (δ/ppm)



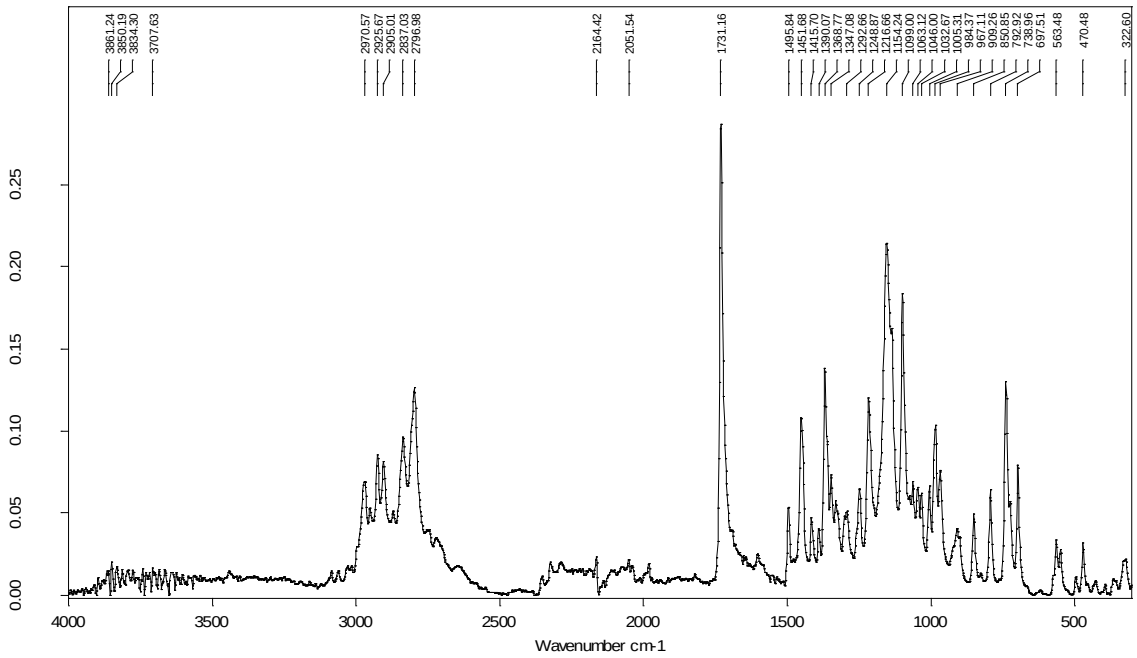
^{13}C-RMN (*J-MODE*) ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

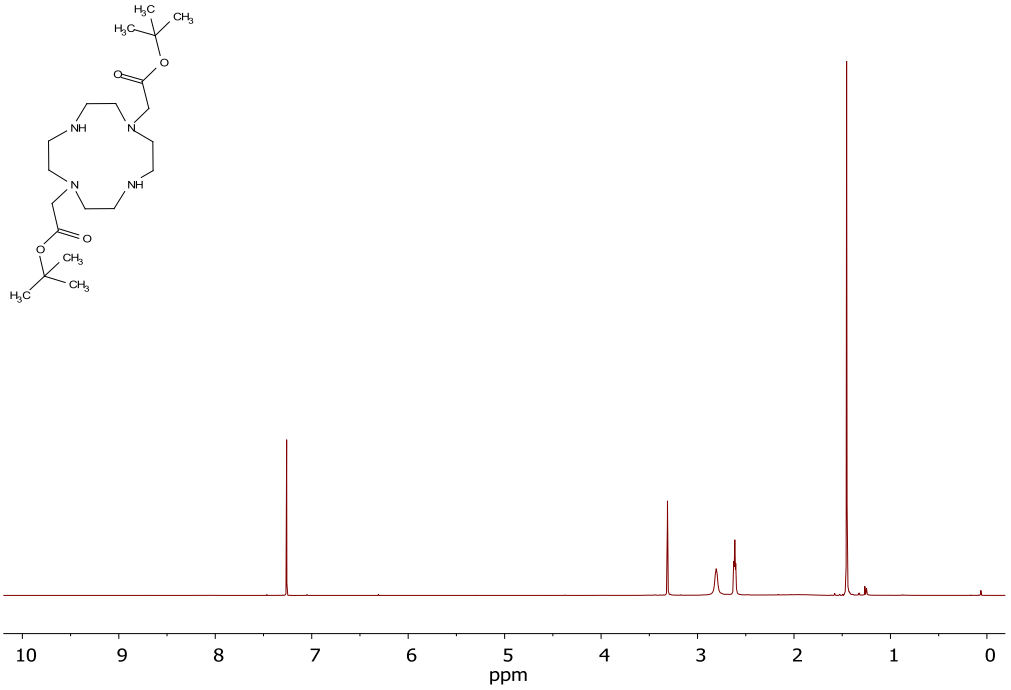


Espectro IR

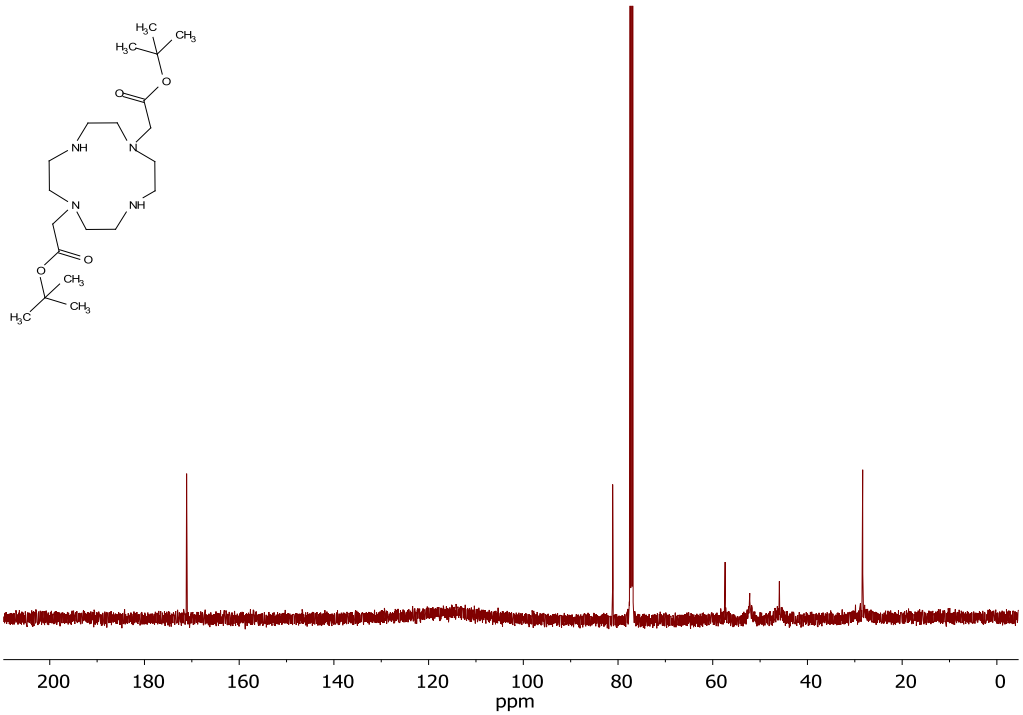


Diacetato de di – tert- butil 2, 2´ - (1, 4, 7, 10 – tetraazaciclododecano – 1, 7 – diil) (**8**)

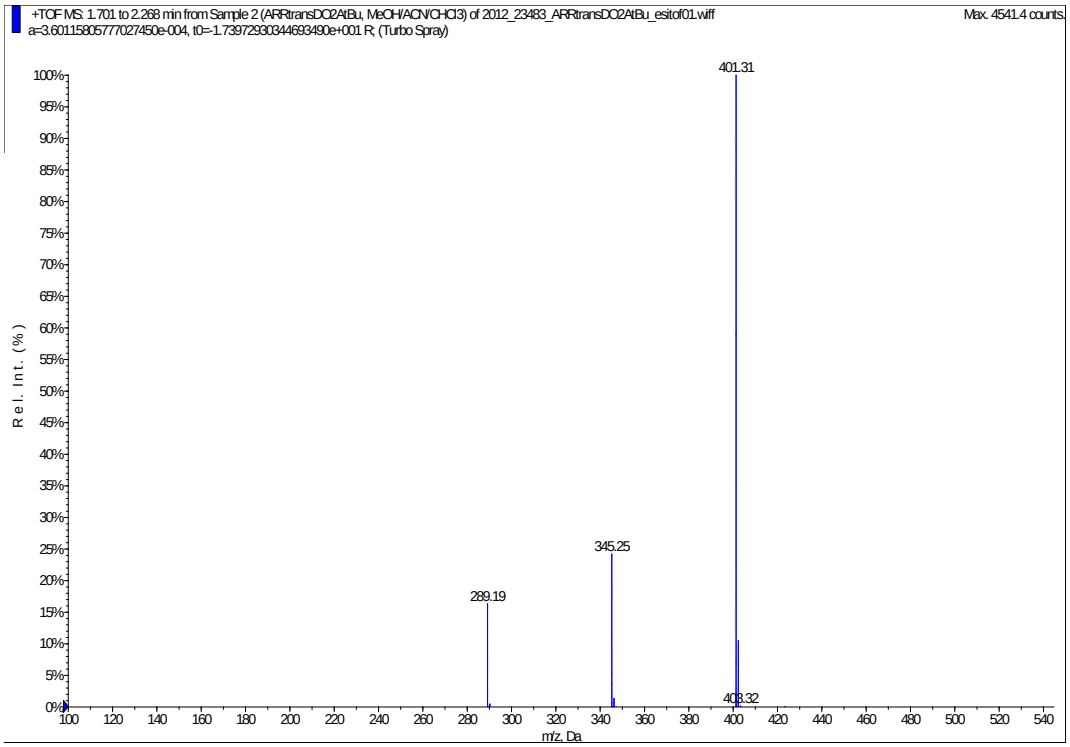
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



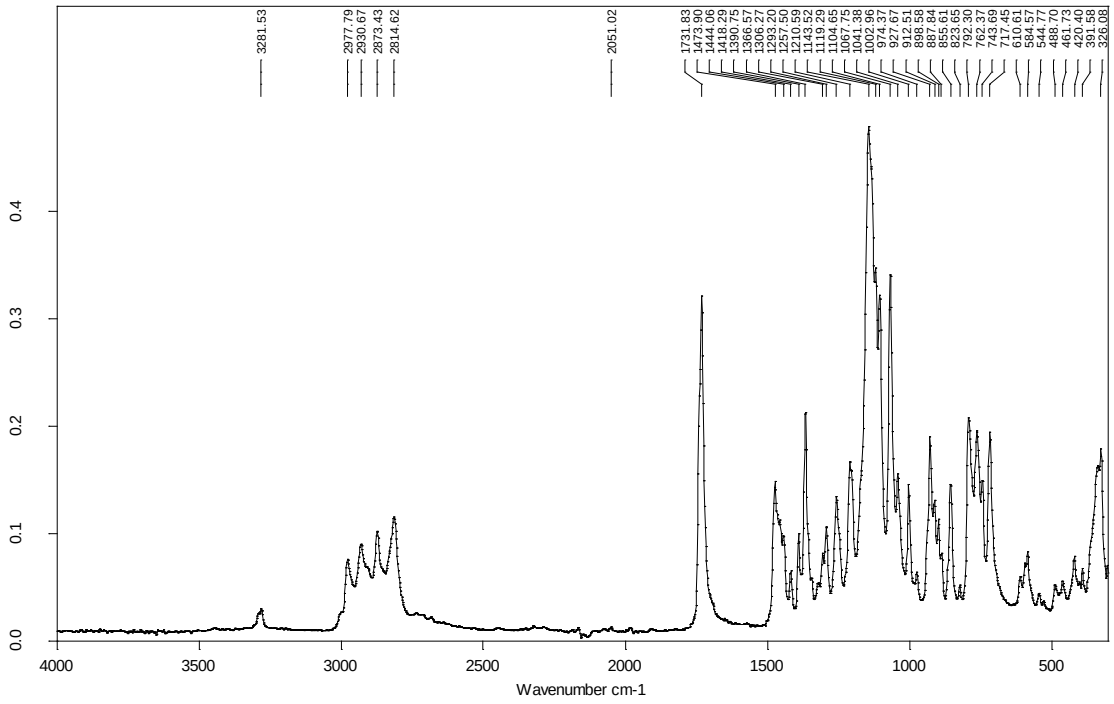
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



Espectro de masas ESI+

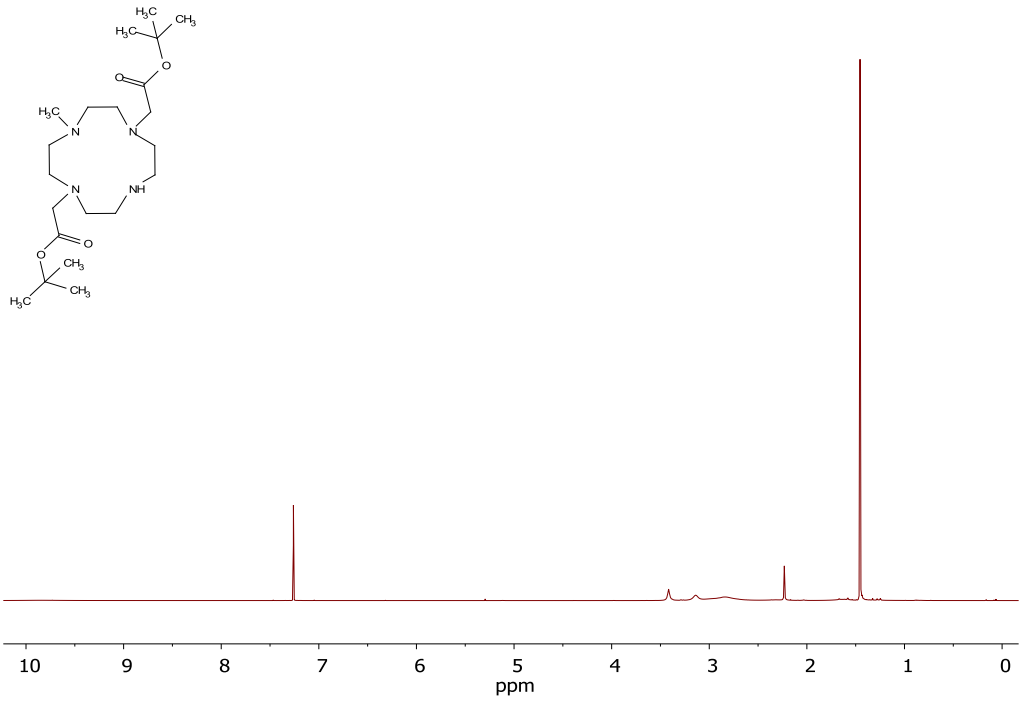


Espectro IR

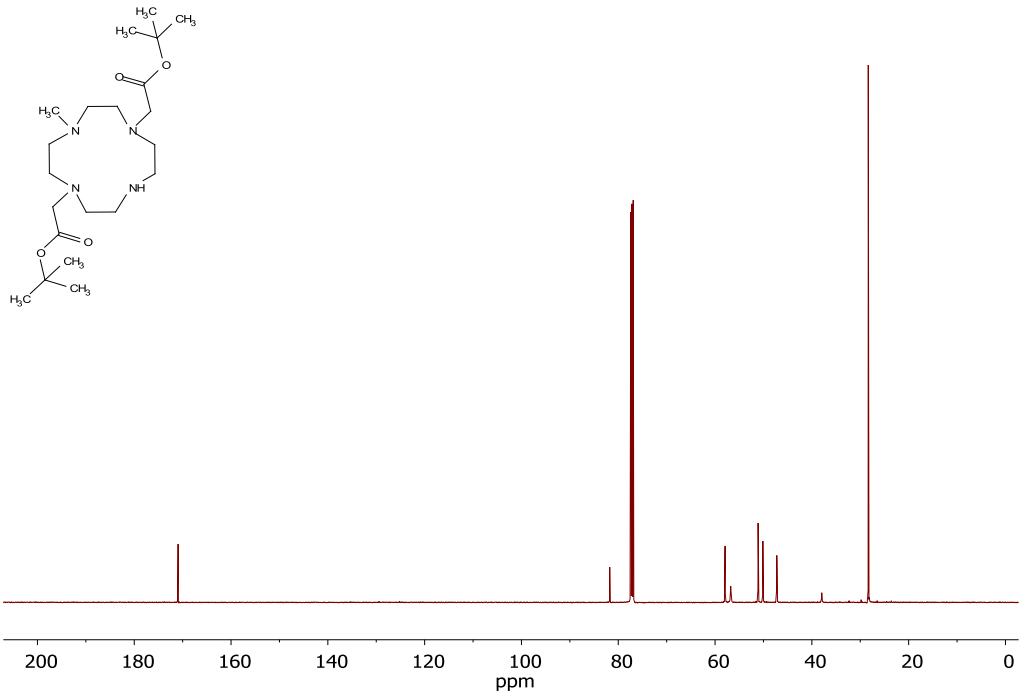


Diacetato de di – tert- butil 2, 2´ - (4 – metil - 1, 4, 7, 10 – tetraazaciclododecano – 1, 7 – diil) (**9**)

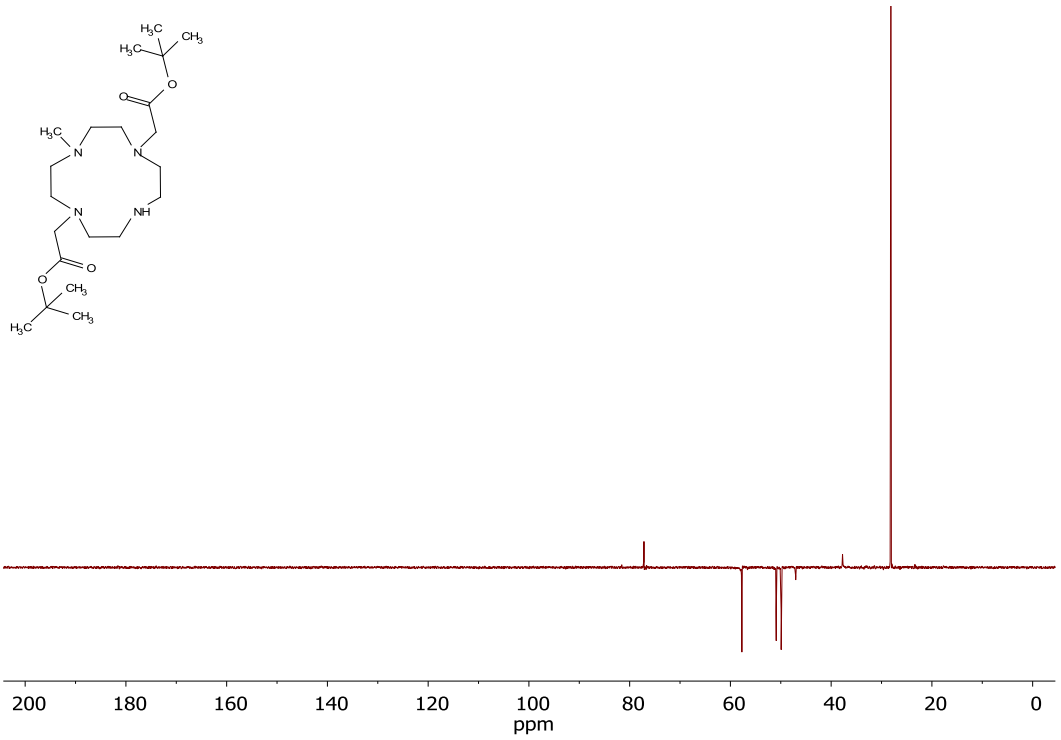
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



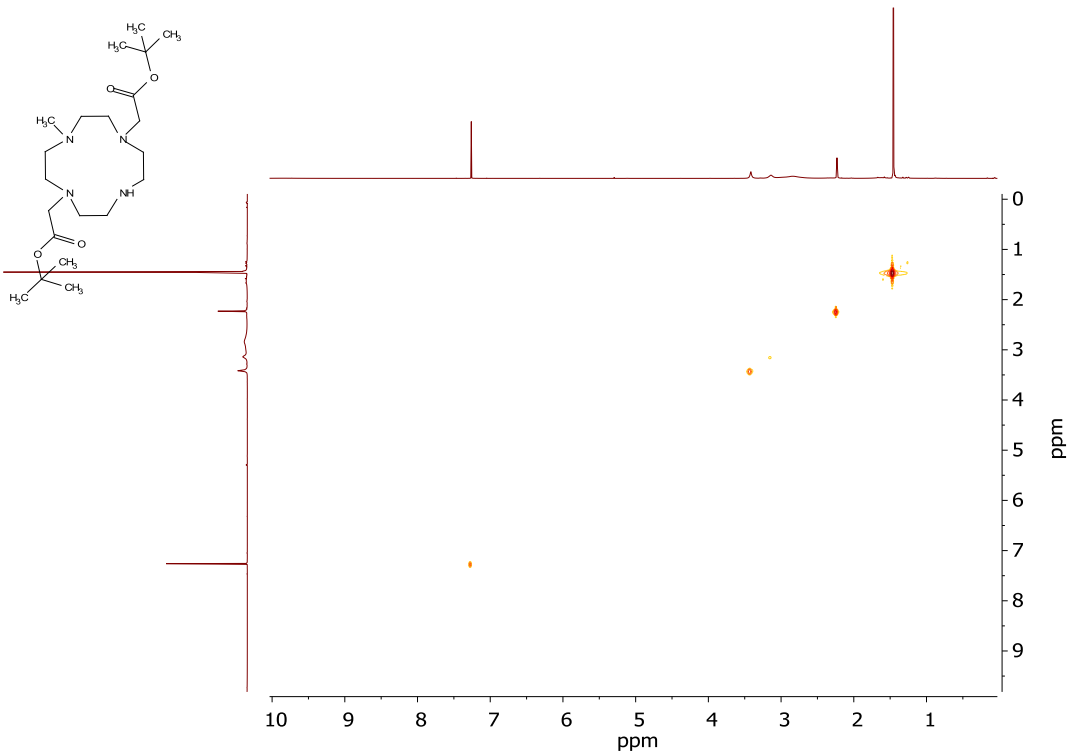
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



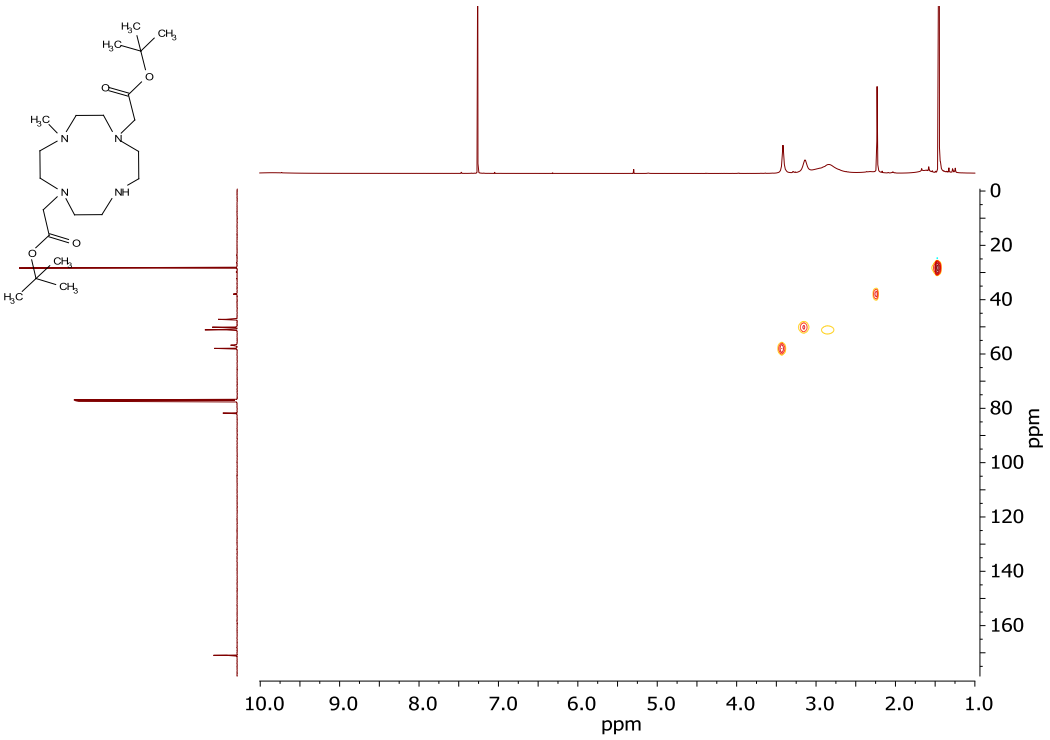
DEPT-RMN ($CDCl_3$) (δ/ppm)



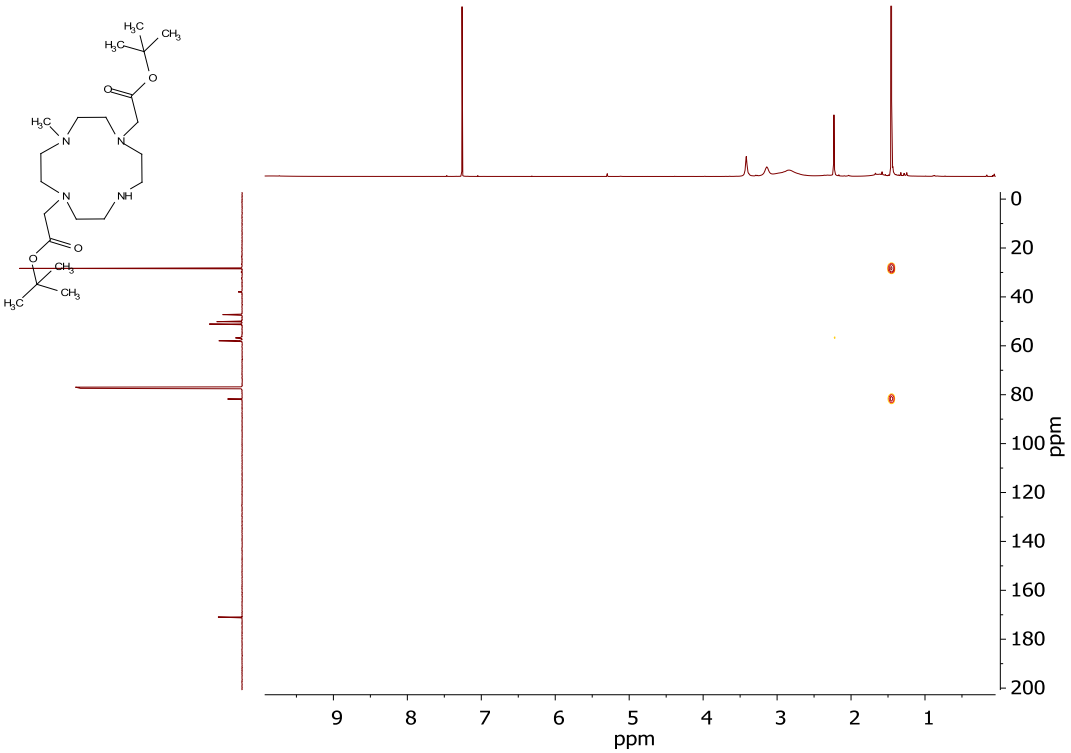
COSY-RMN ($CDCl_3$) (δ/ppm)



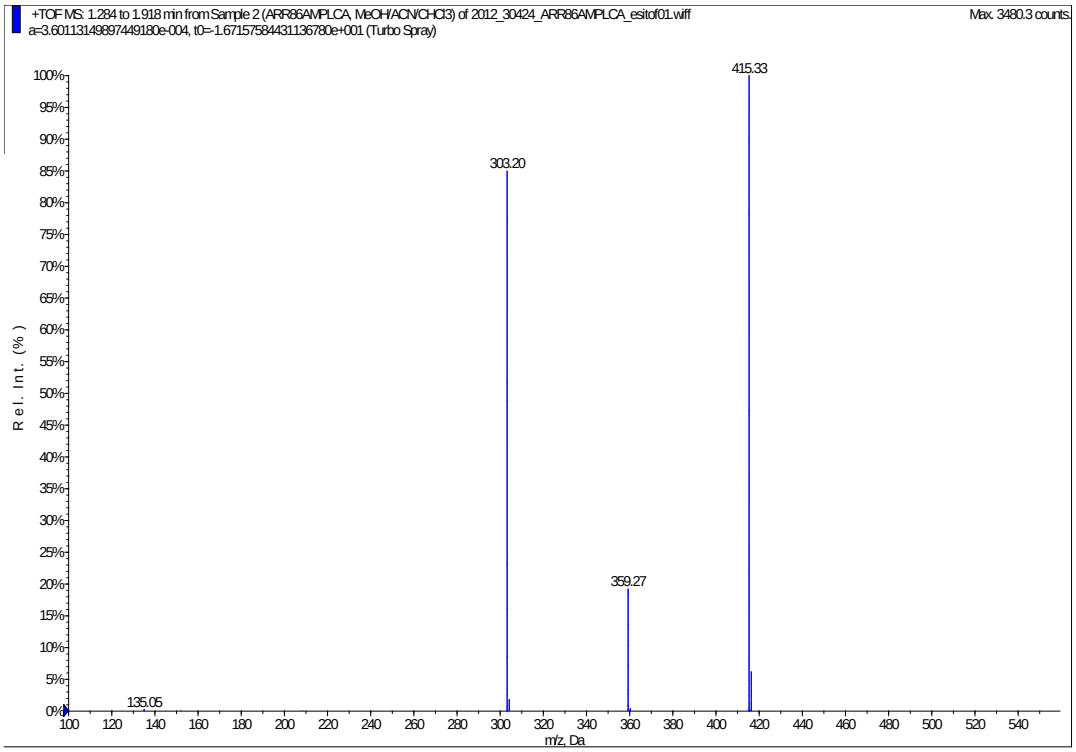
HSQC-RMN ($CDCl_3$) (δ/ppm)



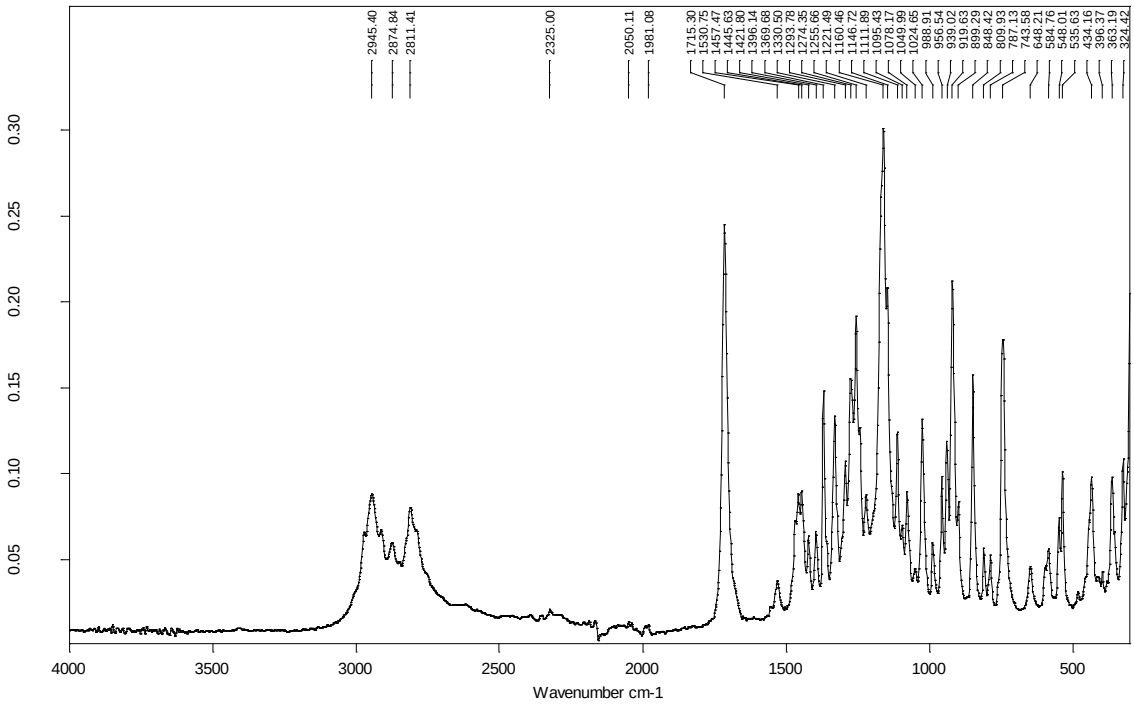
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

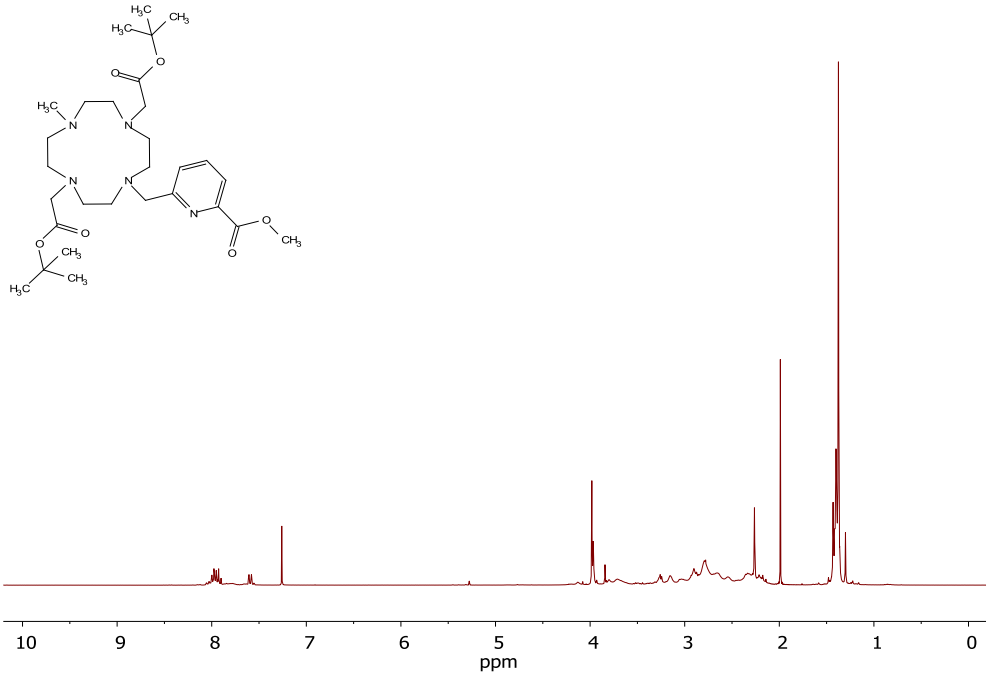


Espectro IR

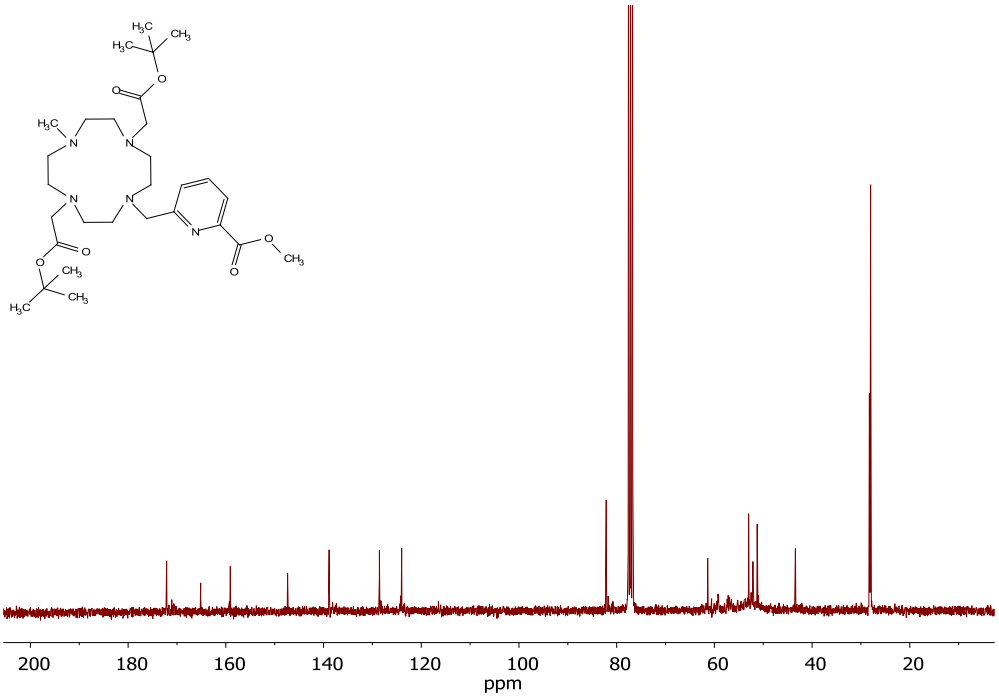


Diacetato de di – tert- butil 2, 2´ - (4 – ((6 – (metoxicarbonil)piridin – 2 il) – 10 – metil - 1, 4, 7, 10 – tetraazaciclododecano – 1, 7 – diil) (**10**)

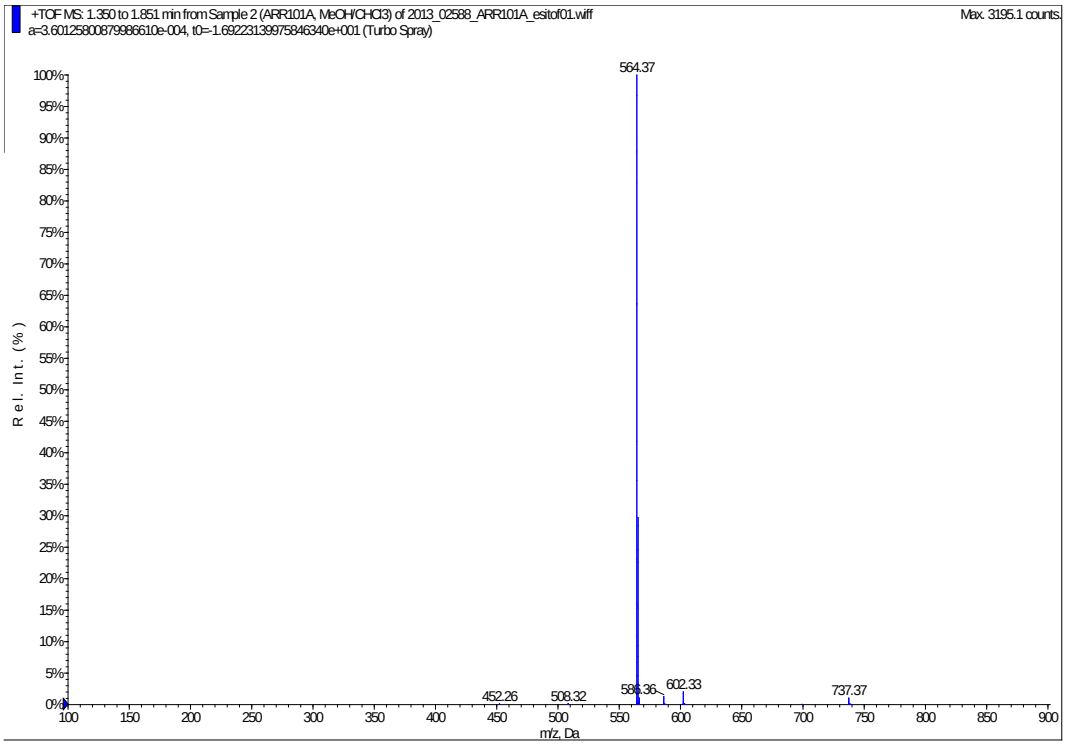
^{1}H-RMN ($CDCl_3$, 300 MHz) (δ/ppm)



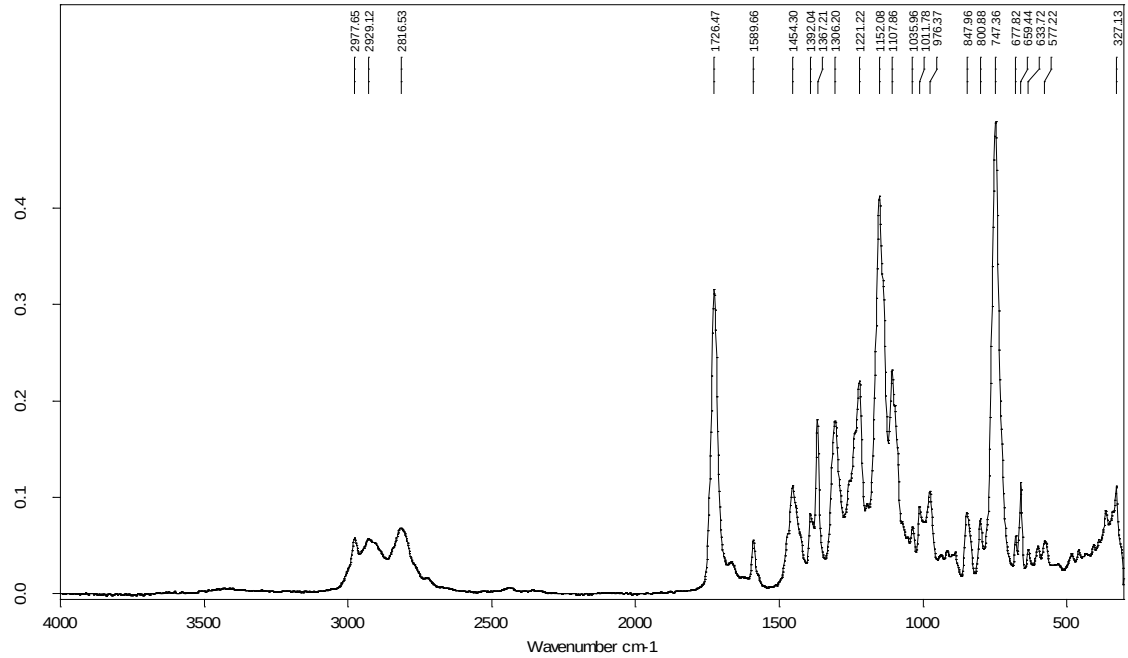
^{13}C-RMN ($CDCl_3$, 75,5 MHz) (δ/ppm)



Espectro de masas ESI+

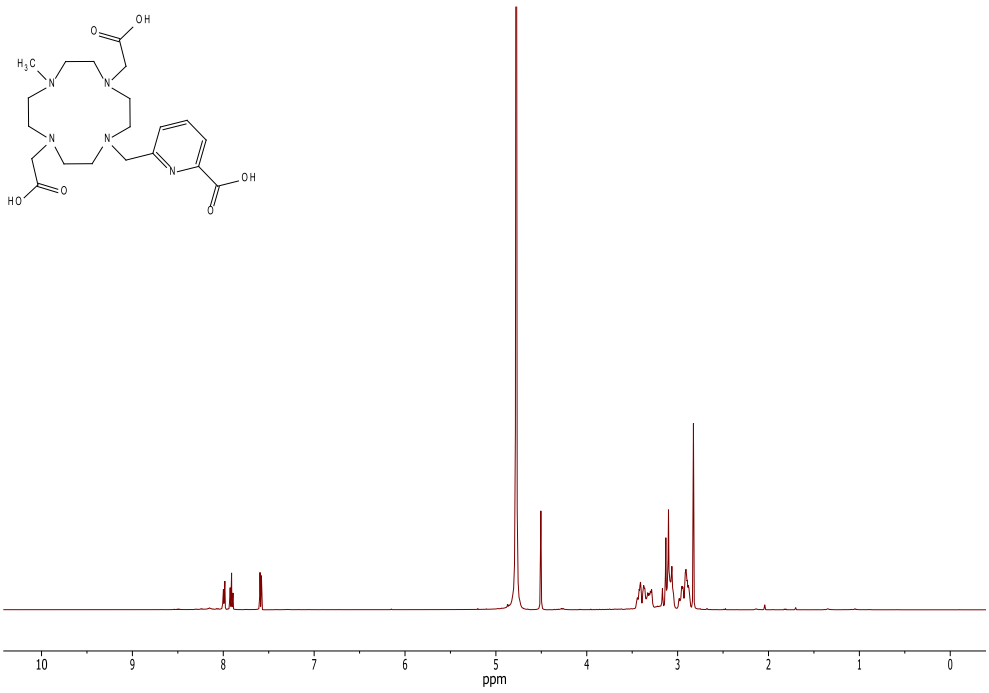


Espectro IR

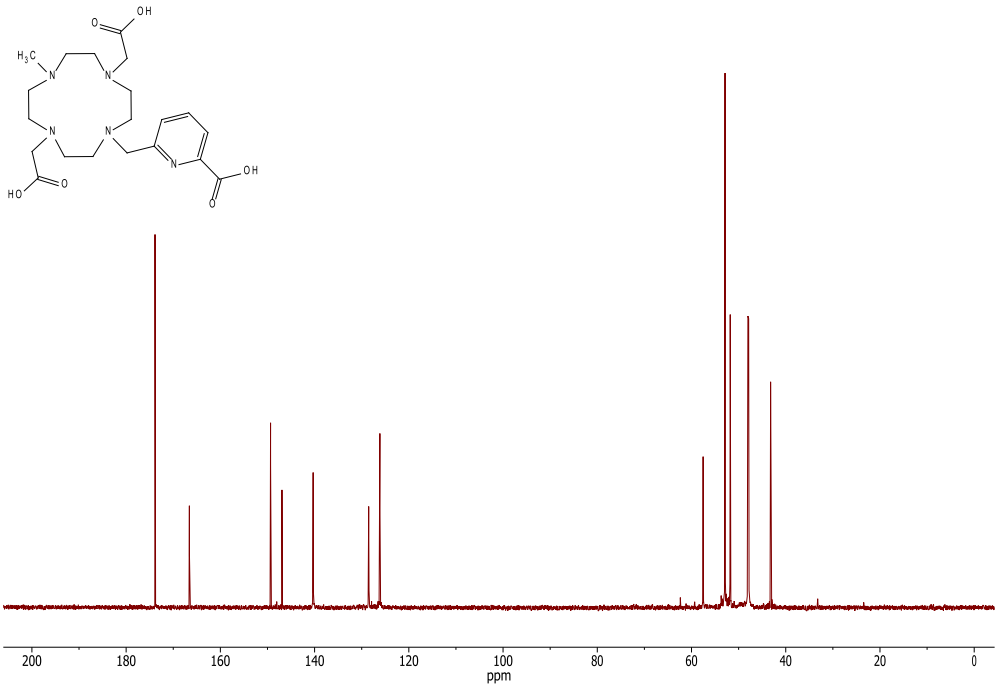


Ácido 2, 2´ - (4 – ((6 –carboxipiridin – 2 il)metil) – 10 – metil - 1, 4, 7, 10 – tetraazaciclododecano – 1, 7 – diil) diacético (**1,7-H_3Medo2apa·7HCl·3H_2O**)

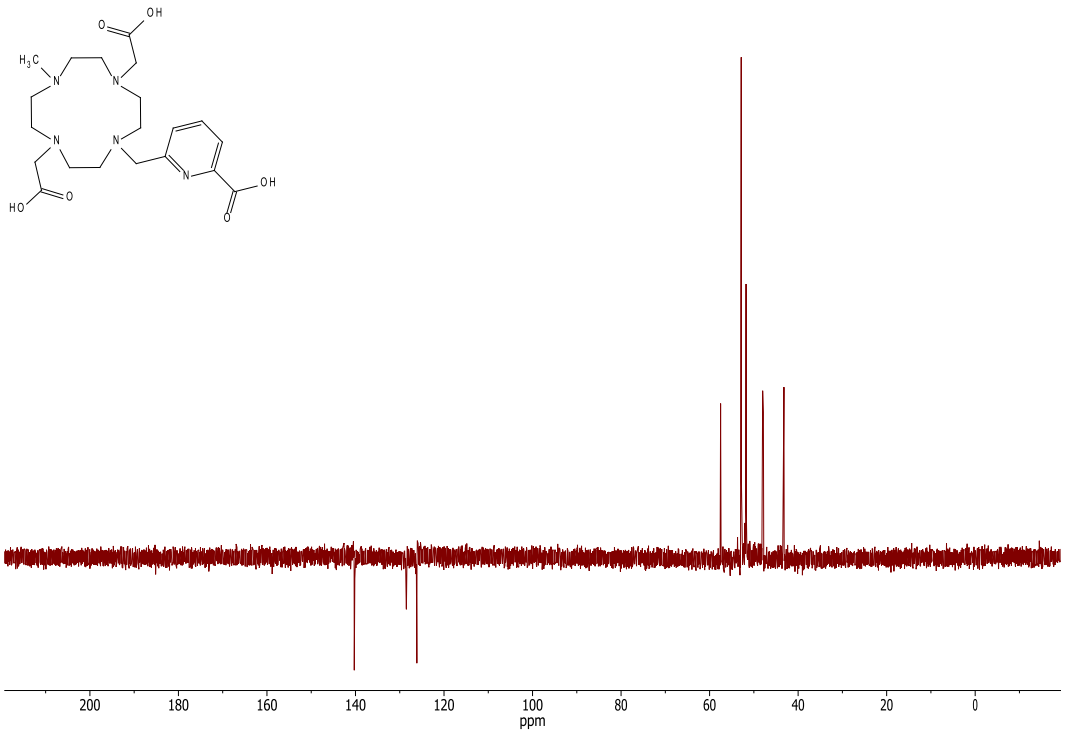
^{1}H-RMN (D_2O, 500 MHz, pD = 0,8) (δ/ppm)



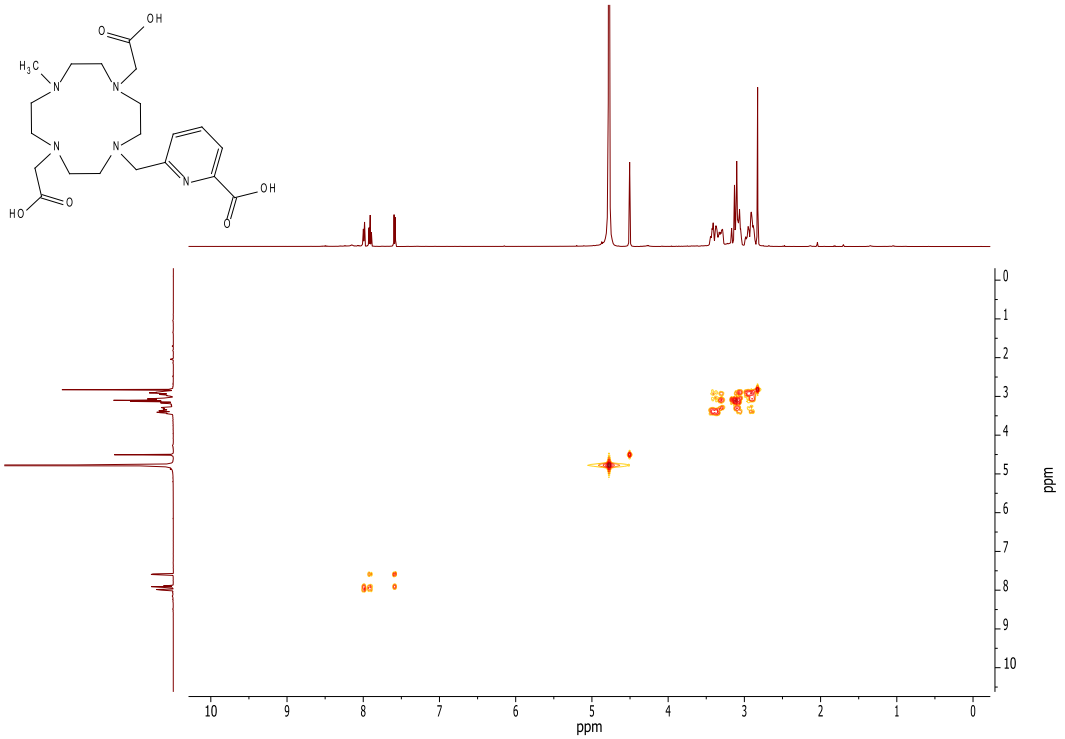
^{13}C-RMN (D_2O, 125,8 MHz, pD = 0,8) (δ/ppm)



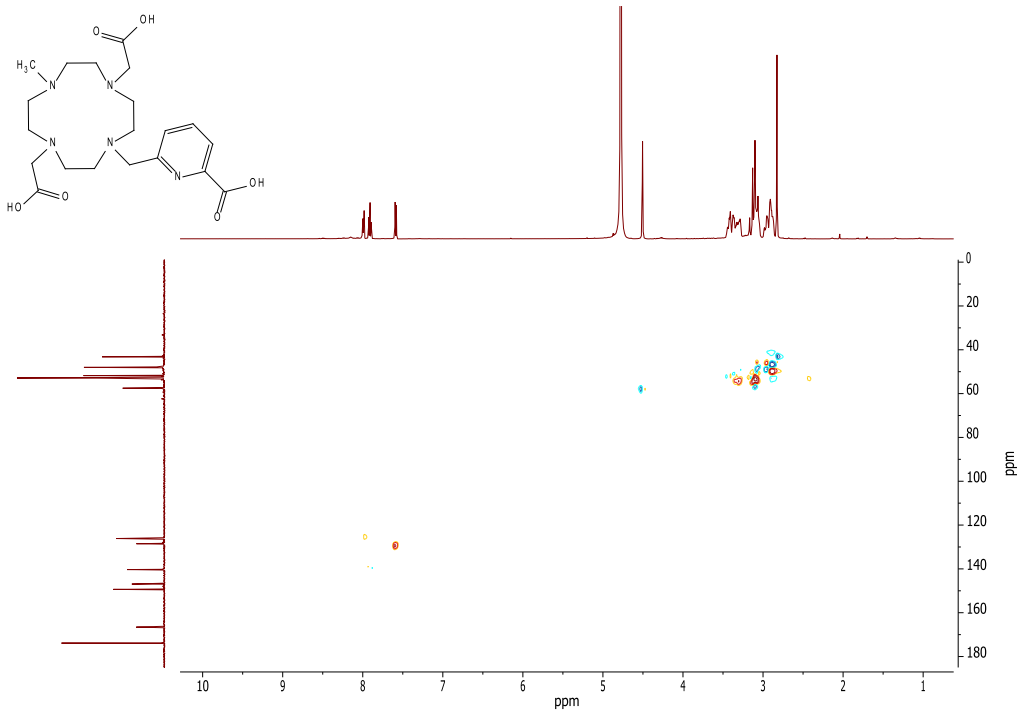
DEPT-RMN (D_2O, pD = 0,8) (δ/ppm)



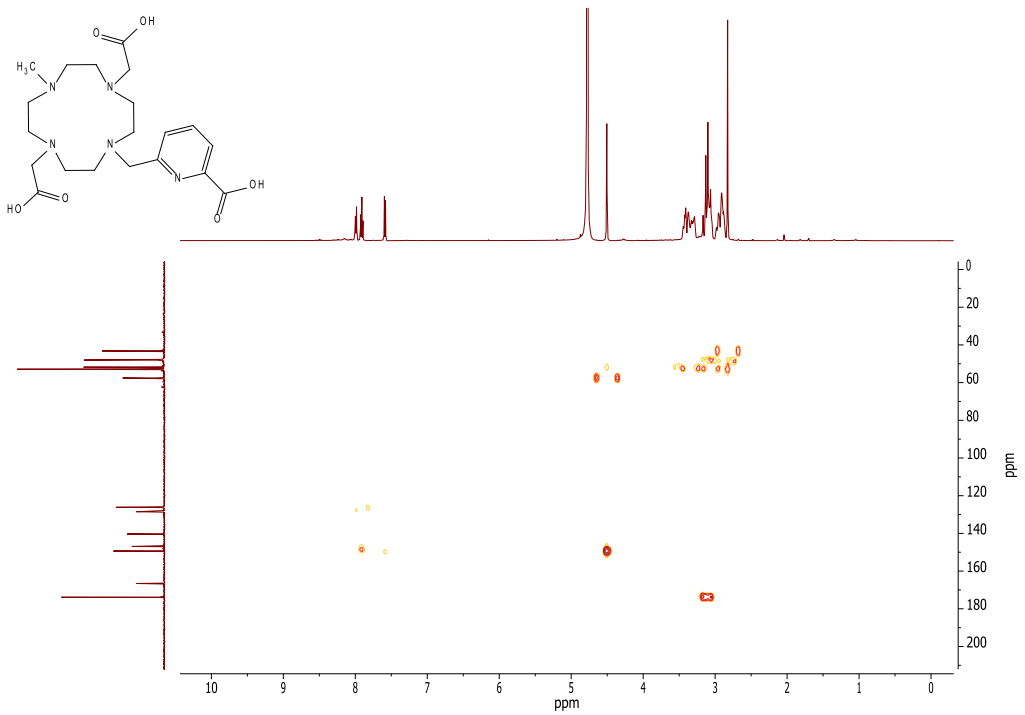
COSY-RMN (D_2O, pD = 0,8) (δ/ppm)



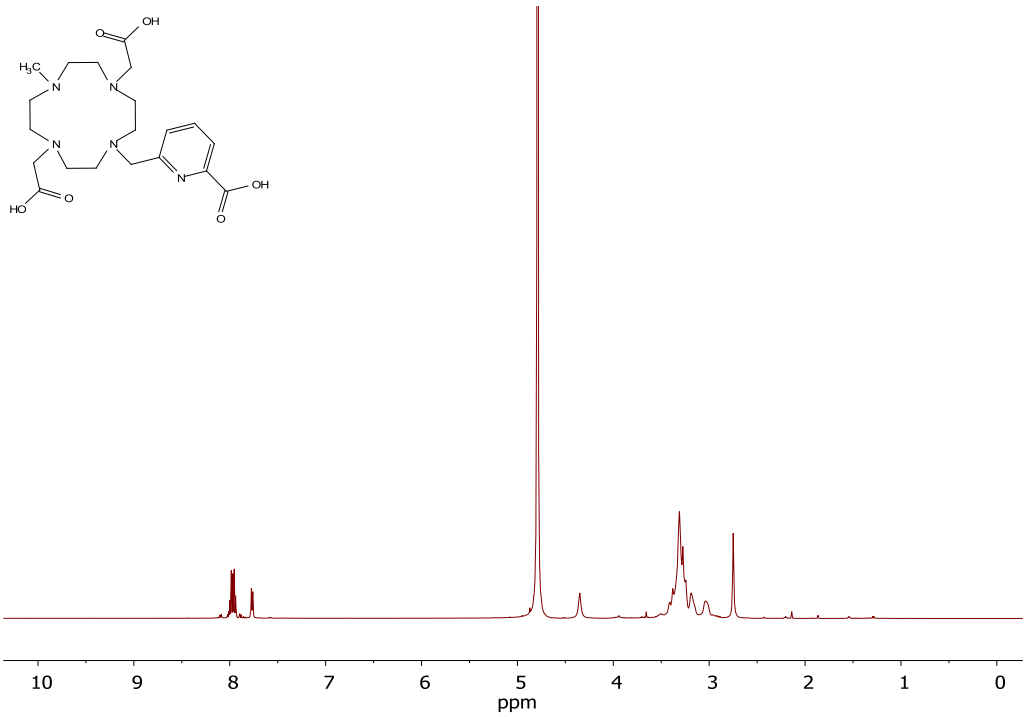
HSQC-RMN (D_2O, pD = 0,8) (δ/ppm)



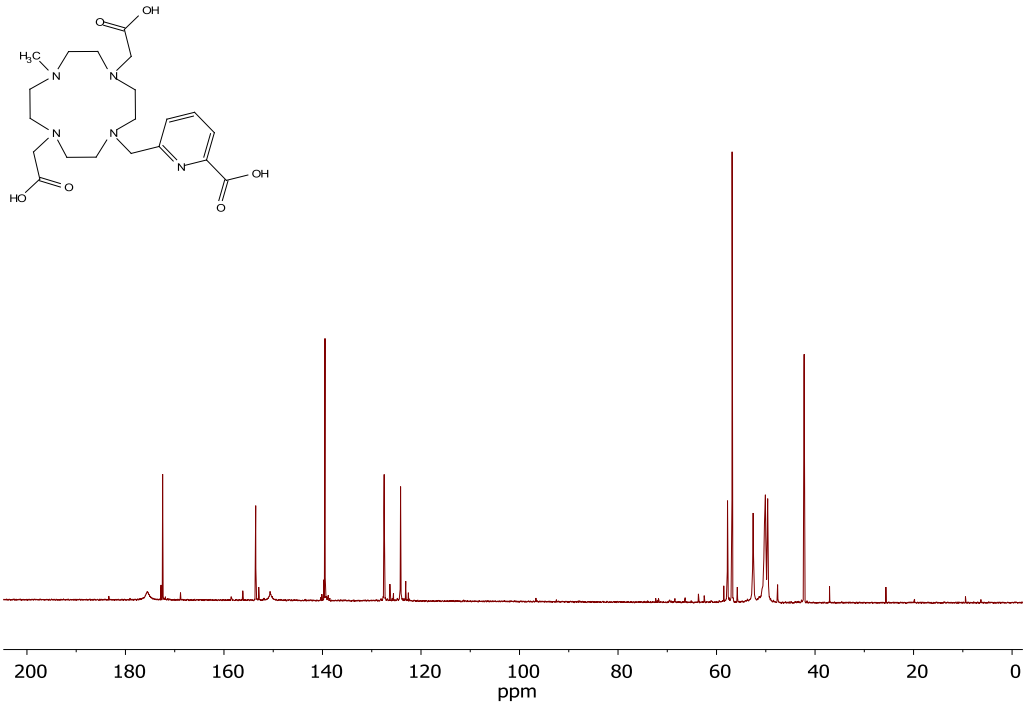
HMBC-RMN (D_2O, pD = 0,8) (δ/ppm)



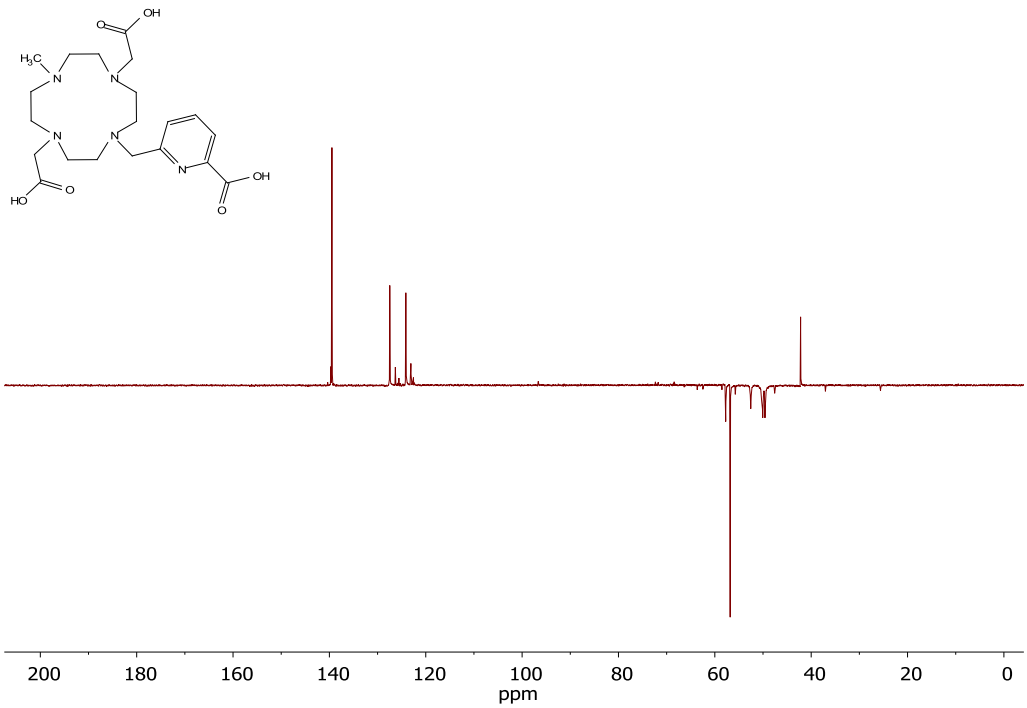
^{1}H-RMN (D_2O, 500 MHz, pD = 7,1) (δ/ppm)



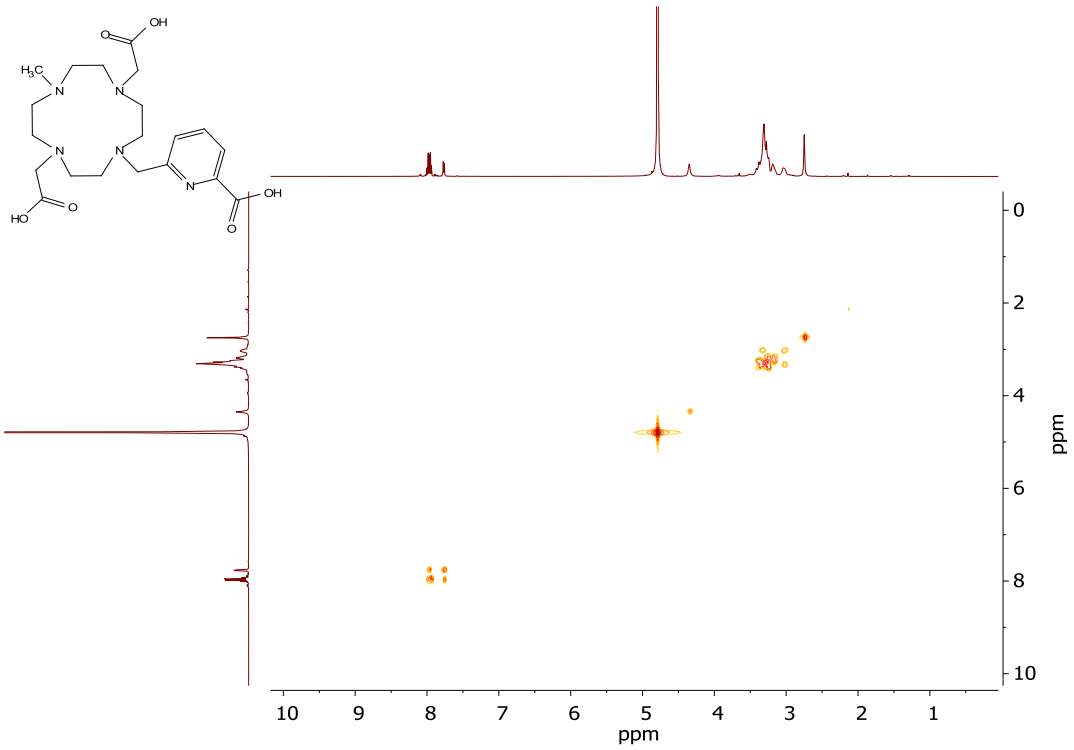
^{13}C-RMN (D_2O, 125,8 MHz, pD = 7,1) (δ/ppm)



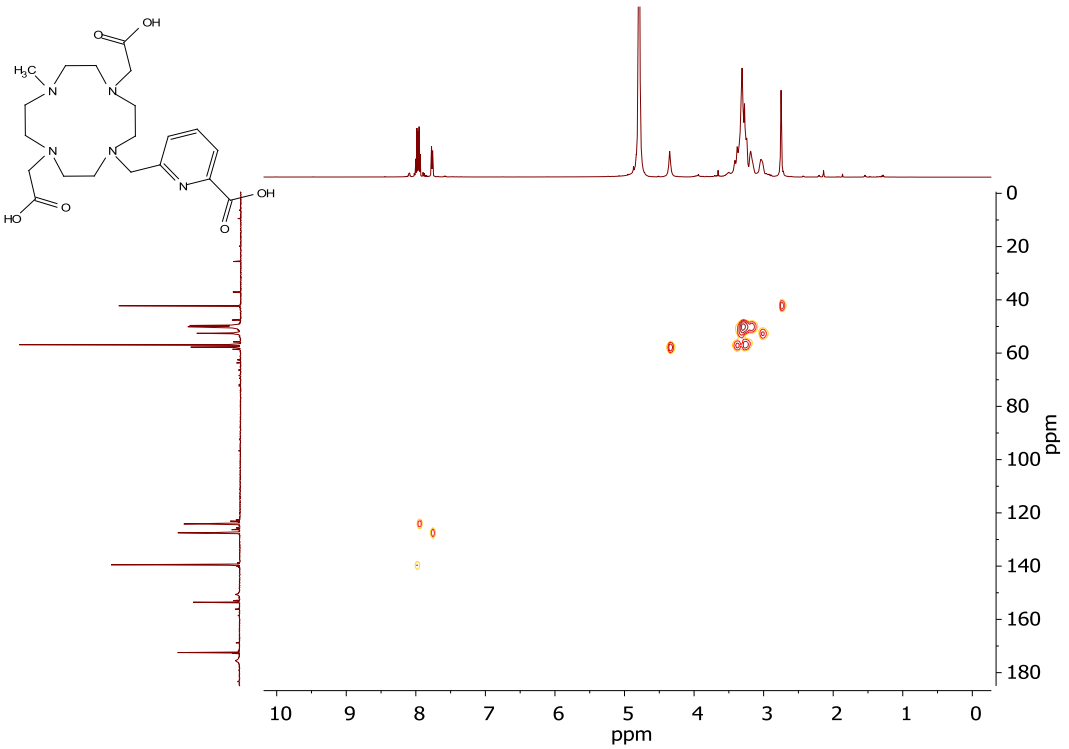
DEPT-RMN (D_2O, pD = 7,1) (δ/ppm)



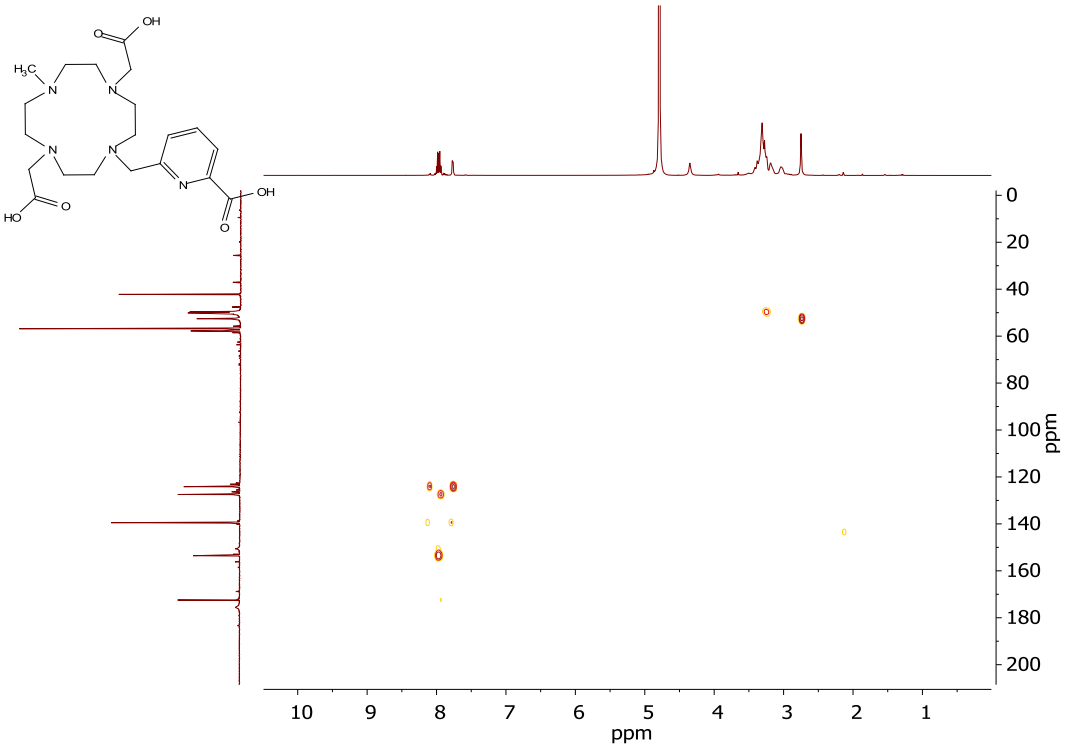
COSY-RMN (D_2O, pD = 7,1) (δ/ppm)



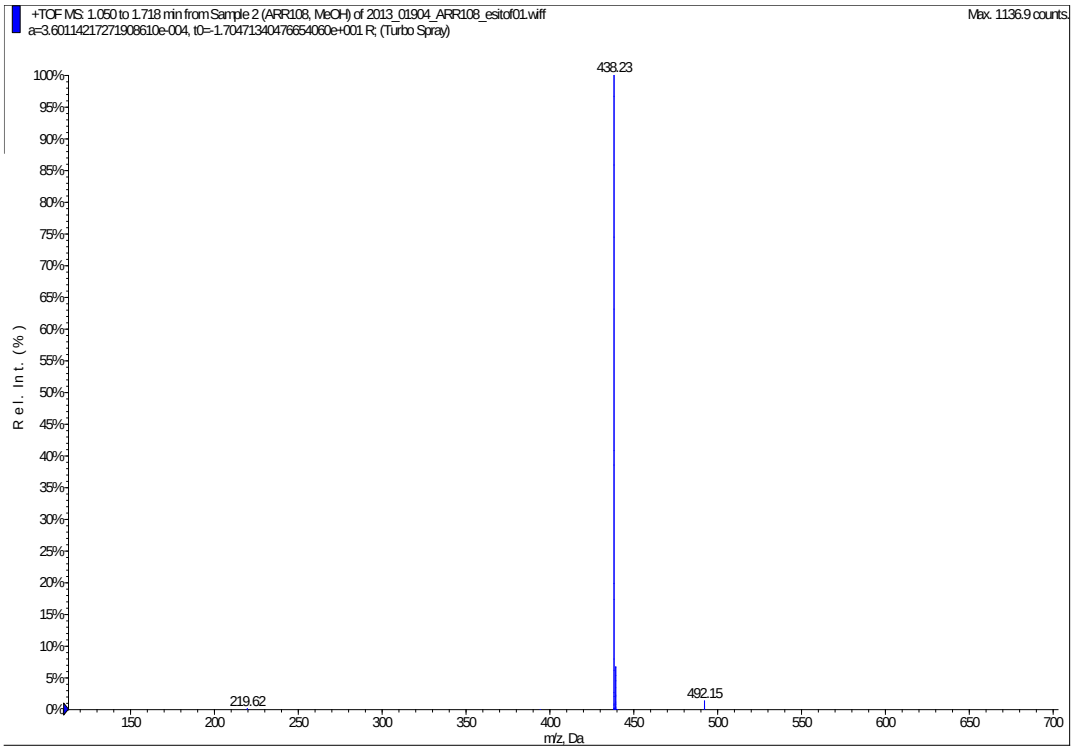
HSQC-RMN (D_2O, pD = 7,1) (δ/ppm)



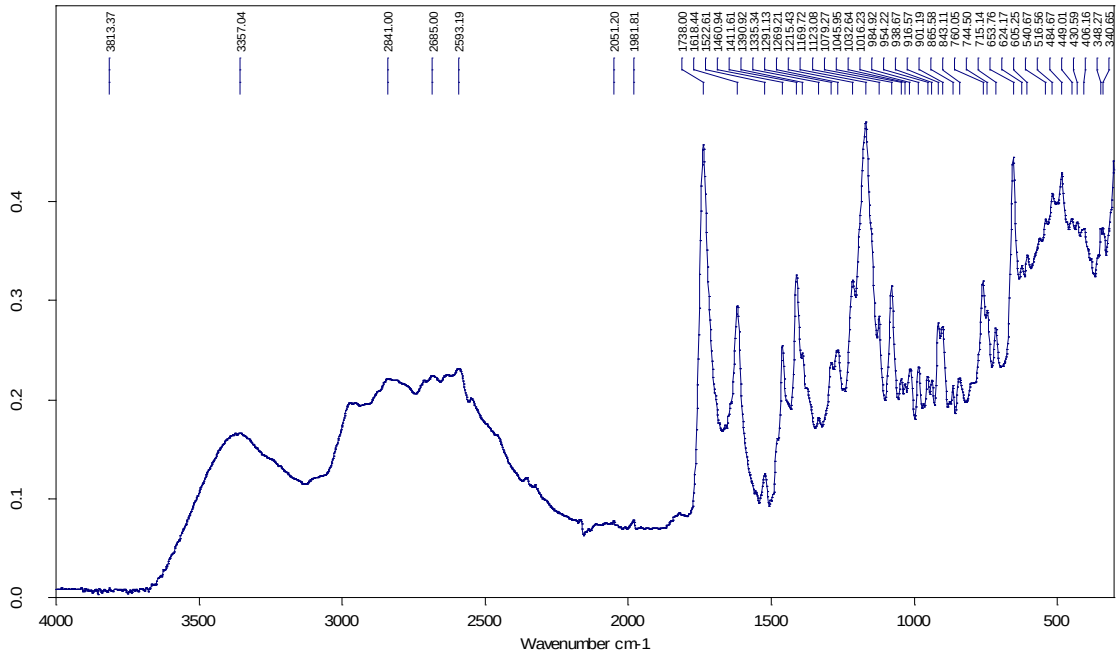
HMBC-RMN (D_2O, pD = 7,1) (δ/ppm)



Espectro de masas ESI+

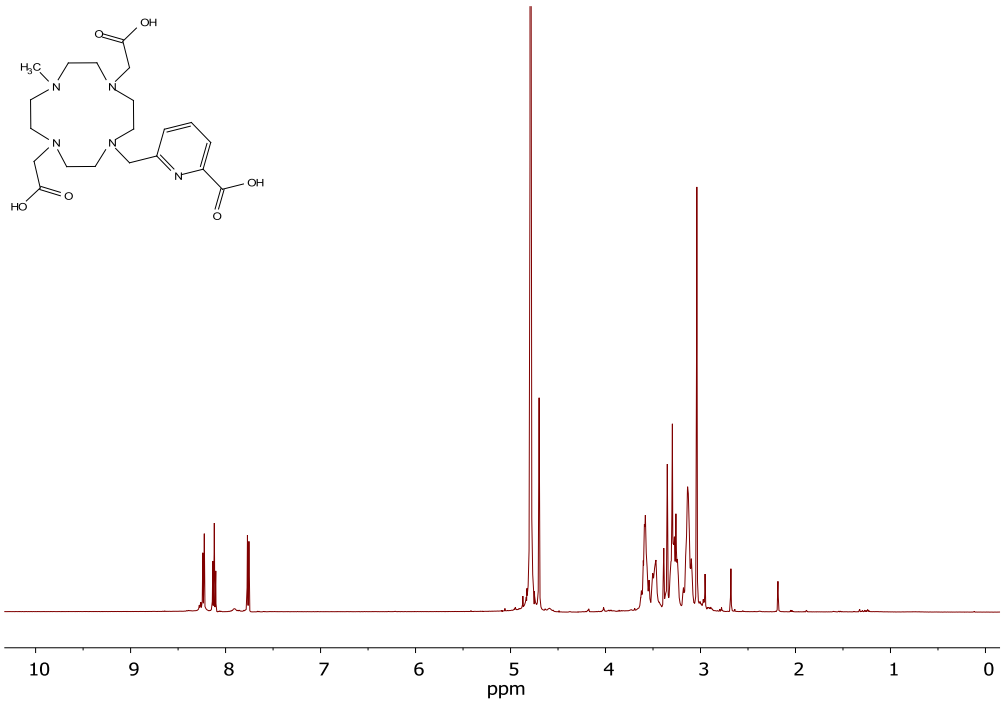


Espectro IR

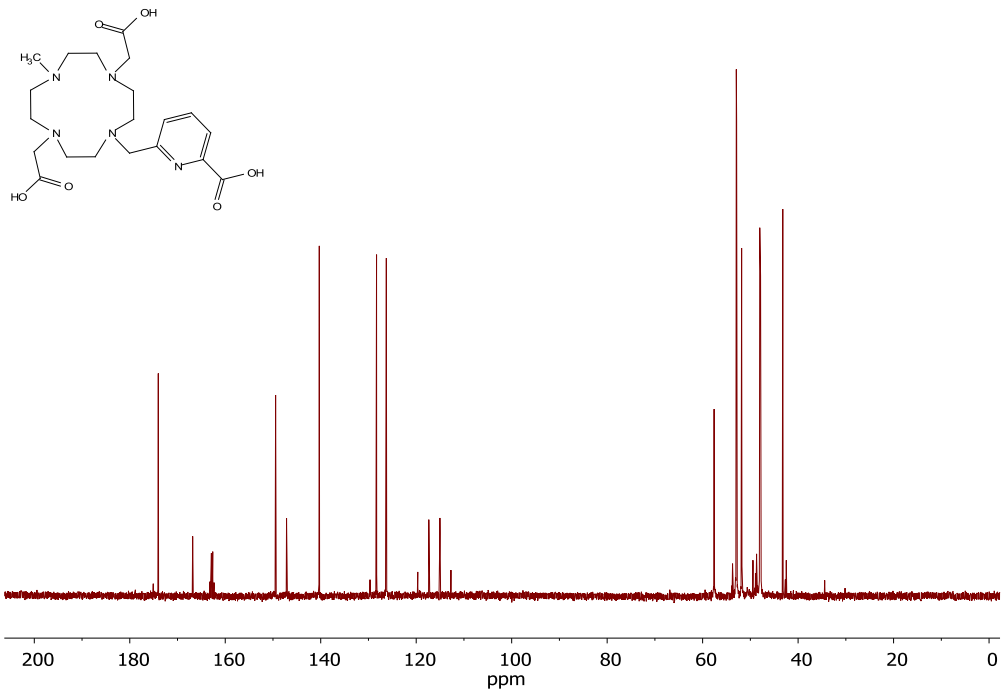


Ácido 2, 2´ - (4 – ((6 –carboxipiridin – 2 il)metil) – 10 – metil - 1, 4, 7, 10 – tetraazaciclododecano – 1, 7 – diil) diacético (**1,7-H_3Medo2apa·8TFA·H_2O**)

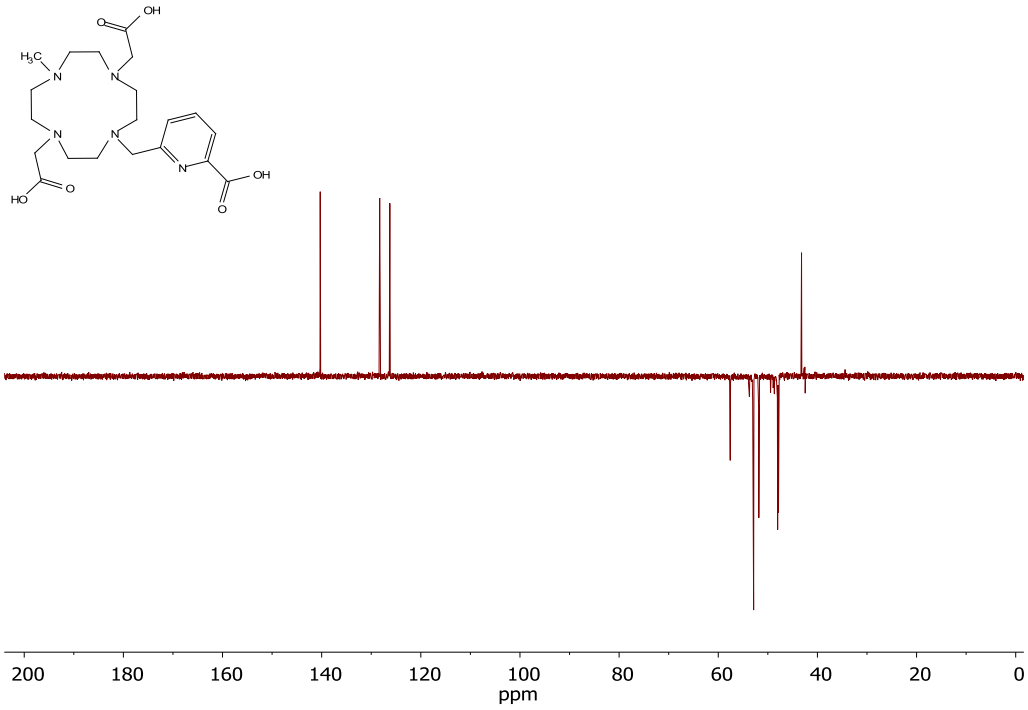
^{1}H-RMN (D_2O, 500 MHz, pD = 1,2) (δ/ppm)



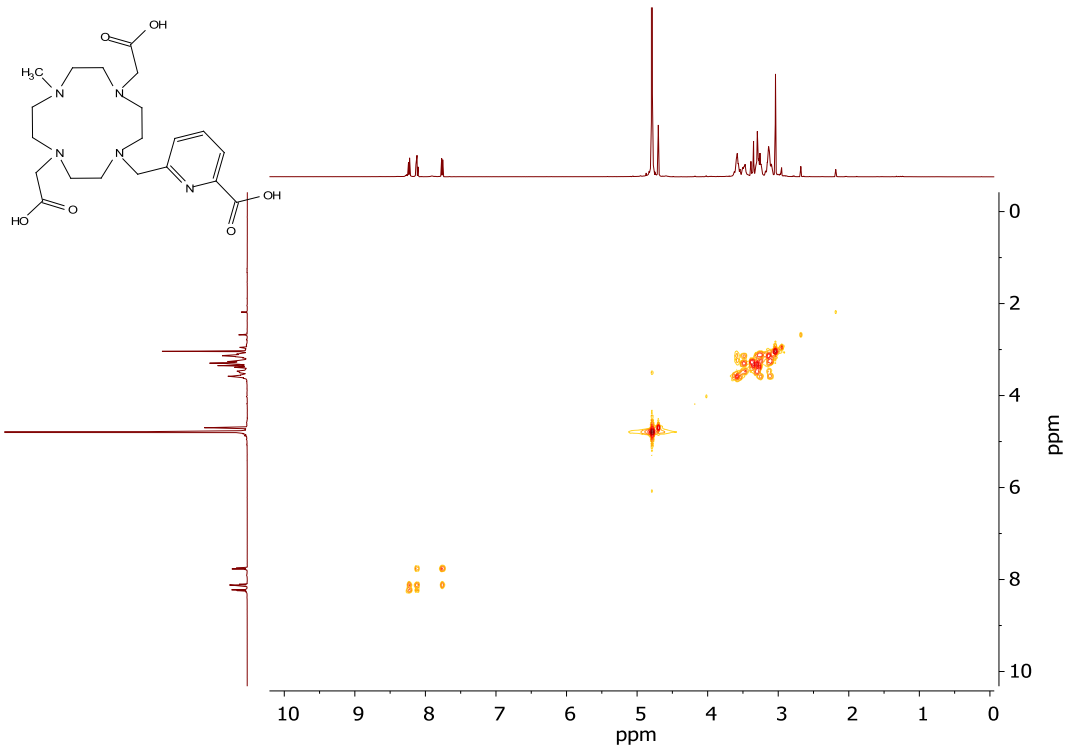
^{13}C-RMN (D_2O, 125,8 MHz, pD = 1,2) (δ/ppm)



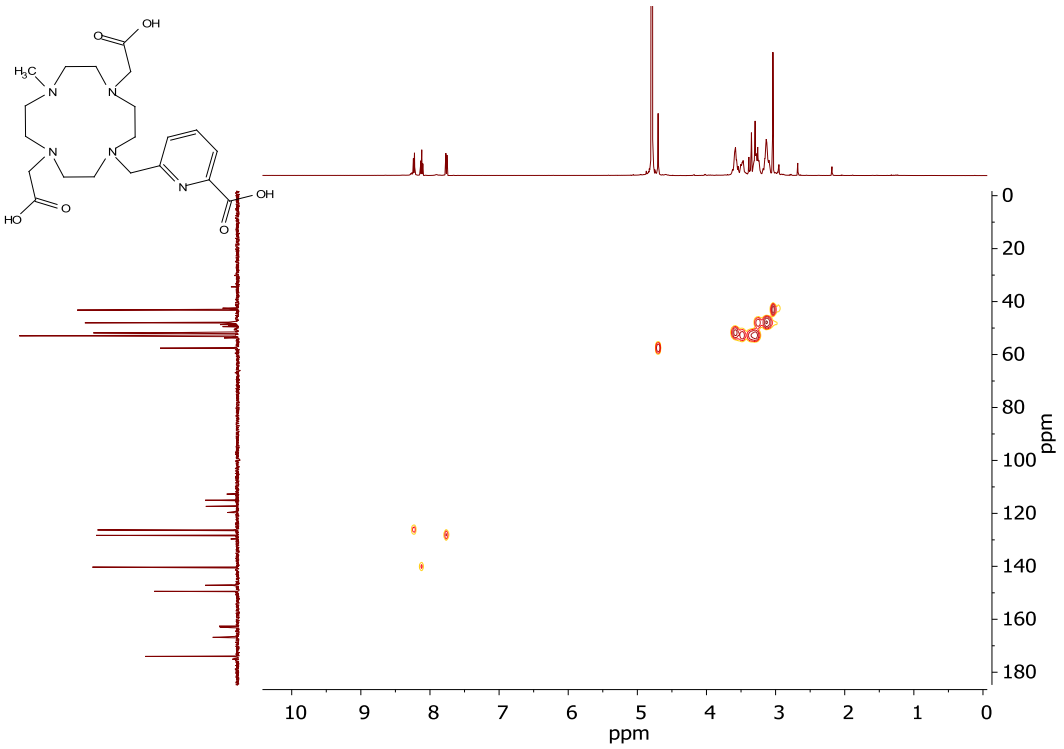
DEPT-RMN (D_2O, pD = 1,2) (δ/ppm)



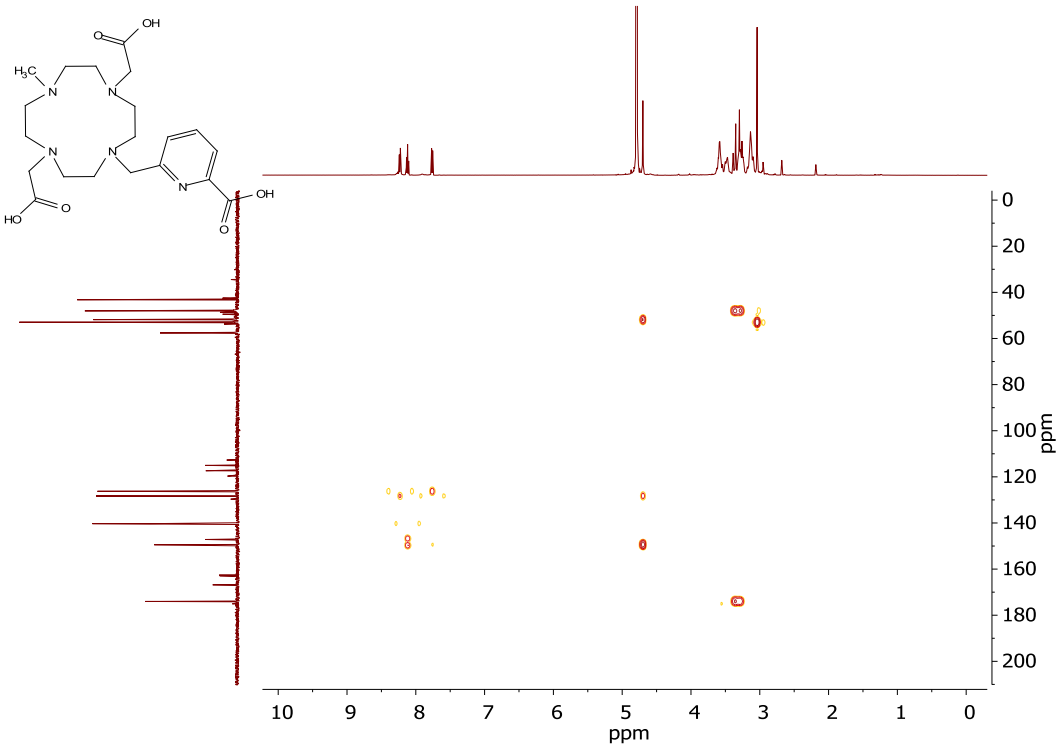
COSY-RMN (D_2O, pD = 1,2) (δ/ppm)



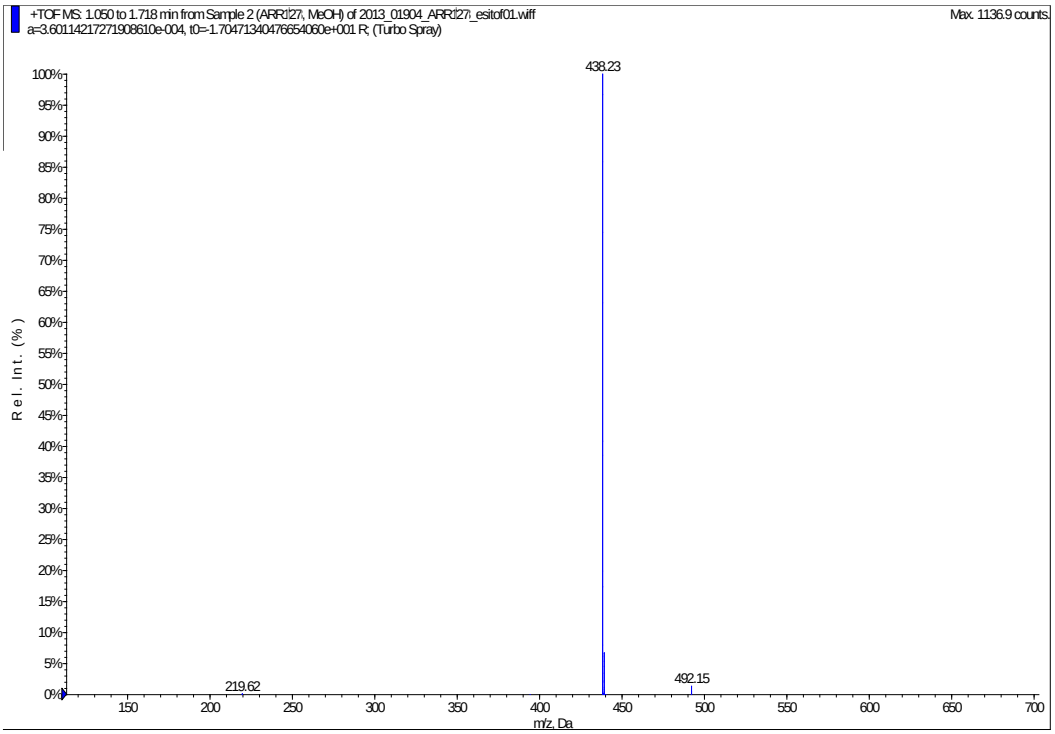
HSQC-RMN (D_2O, pD = 1,2) (δ/ppm)



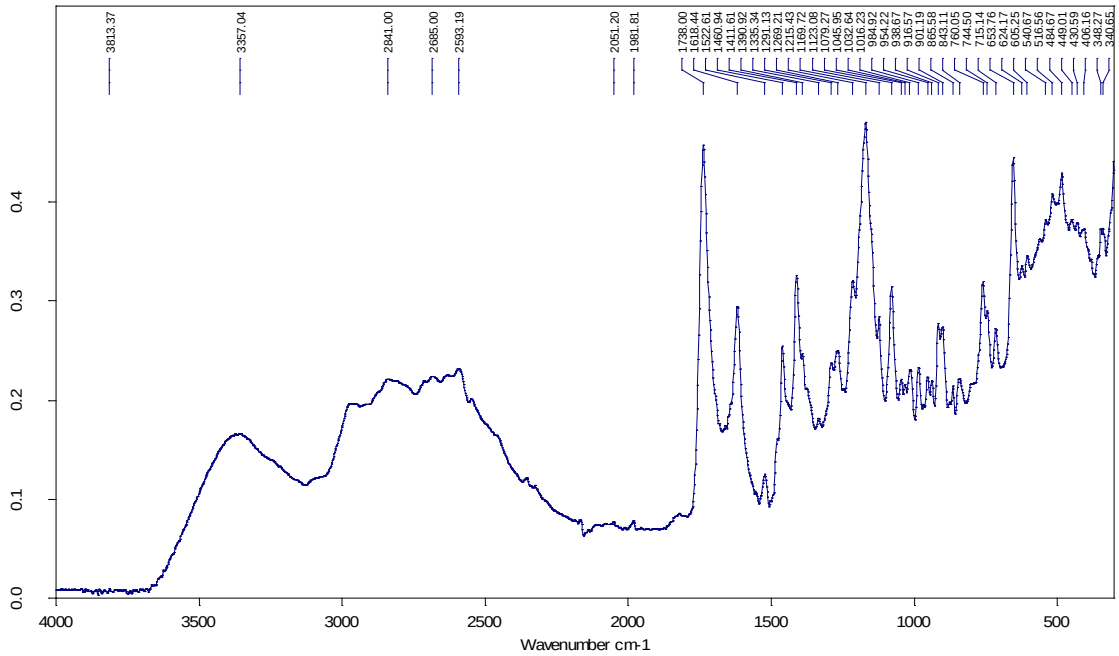
HMBC-RMN (D_2O, pD = 1,2) (δ/ppm)



Espectro de masas ESI+

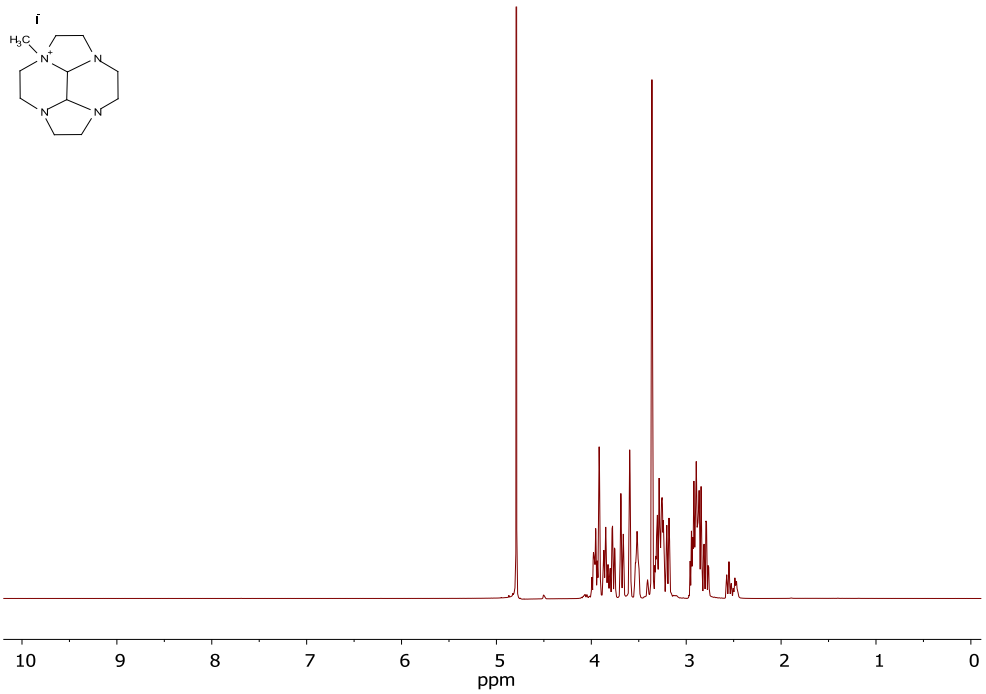


Espectro IR

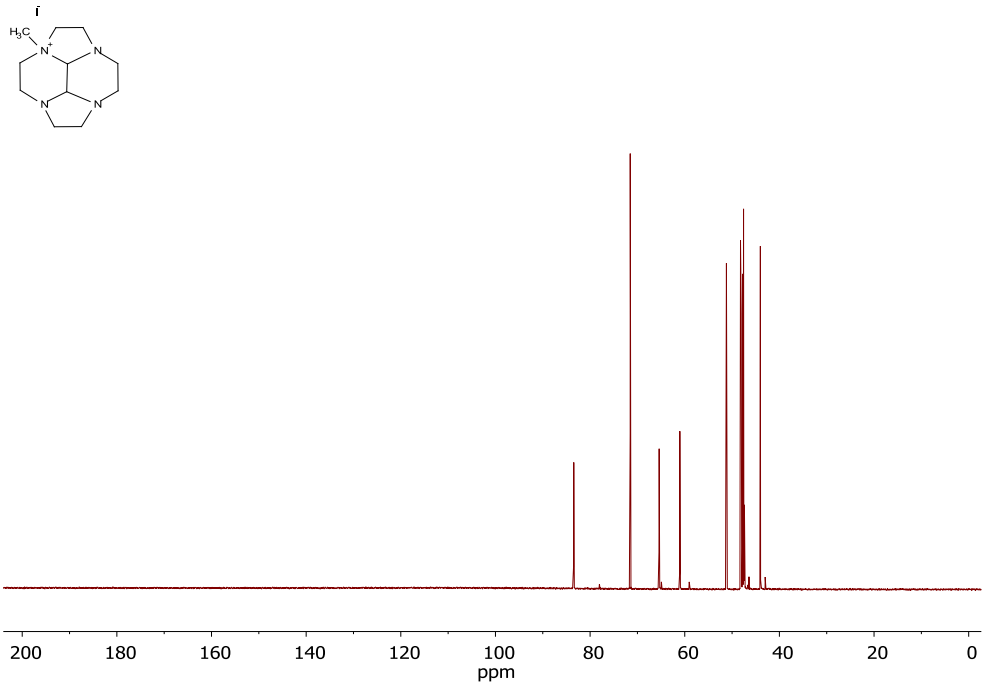


2a - Yoduro de 2a - metildodecahidro – 1H - 2a,4a,6a,8a – tetraazaciclopenta[fg]acenaftileno - yoduro de 1 - metil ciclén glioxal – (**11**)

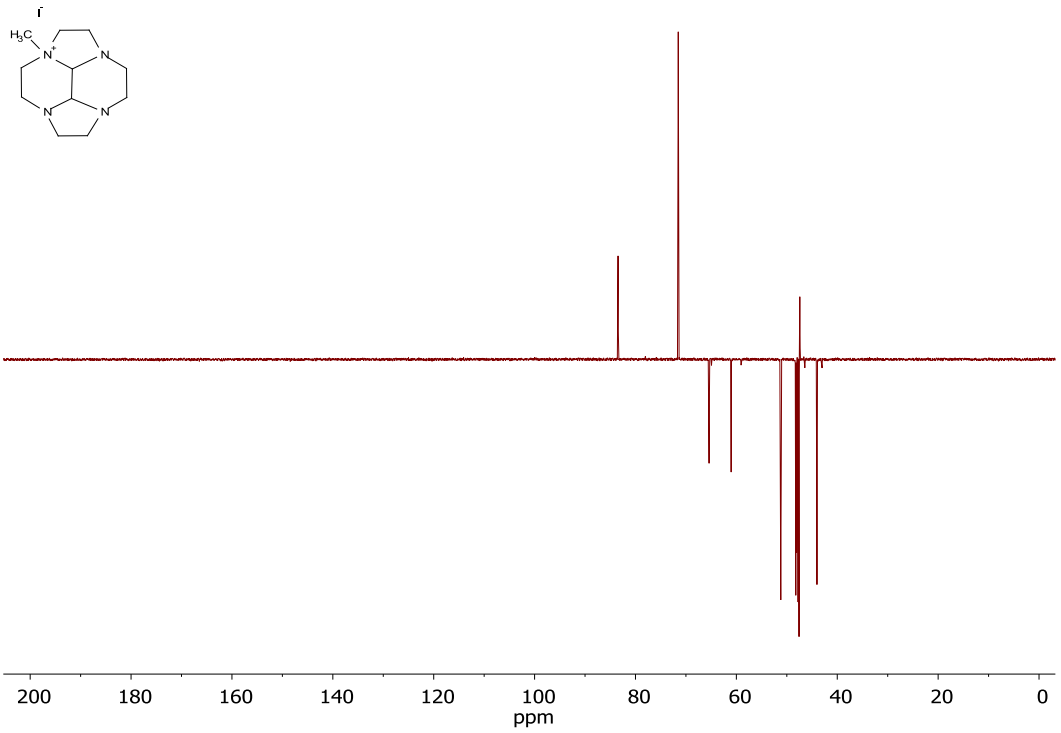
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



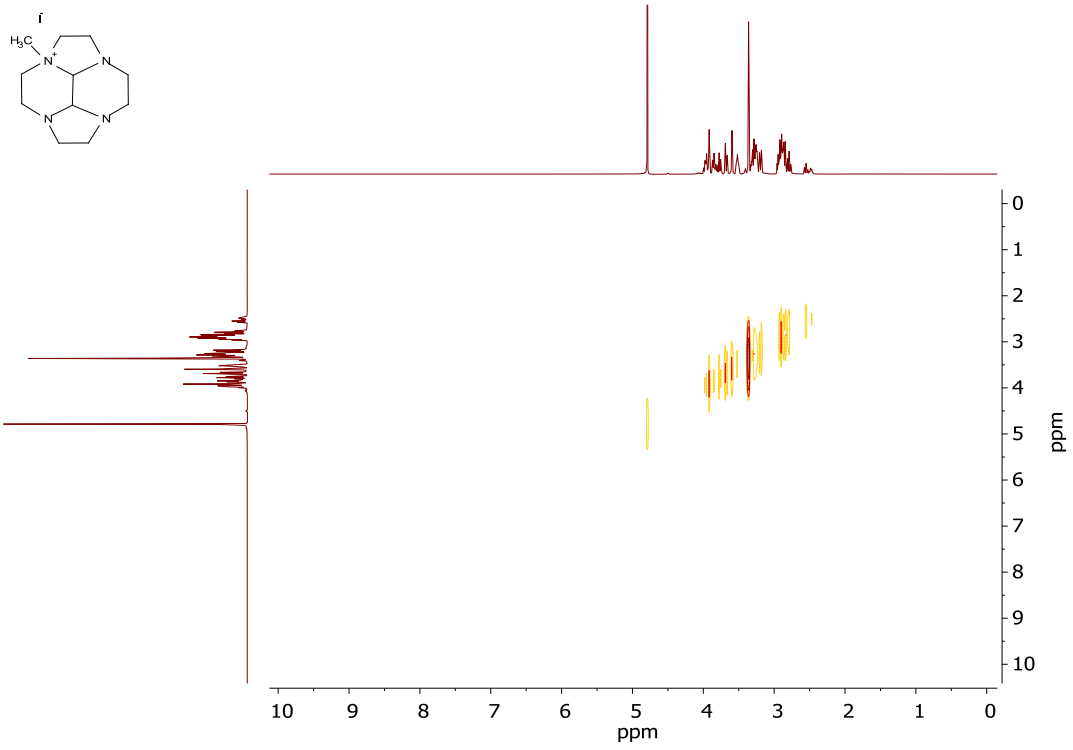
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



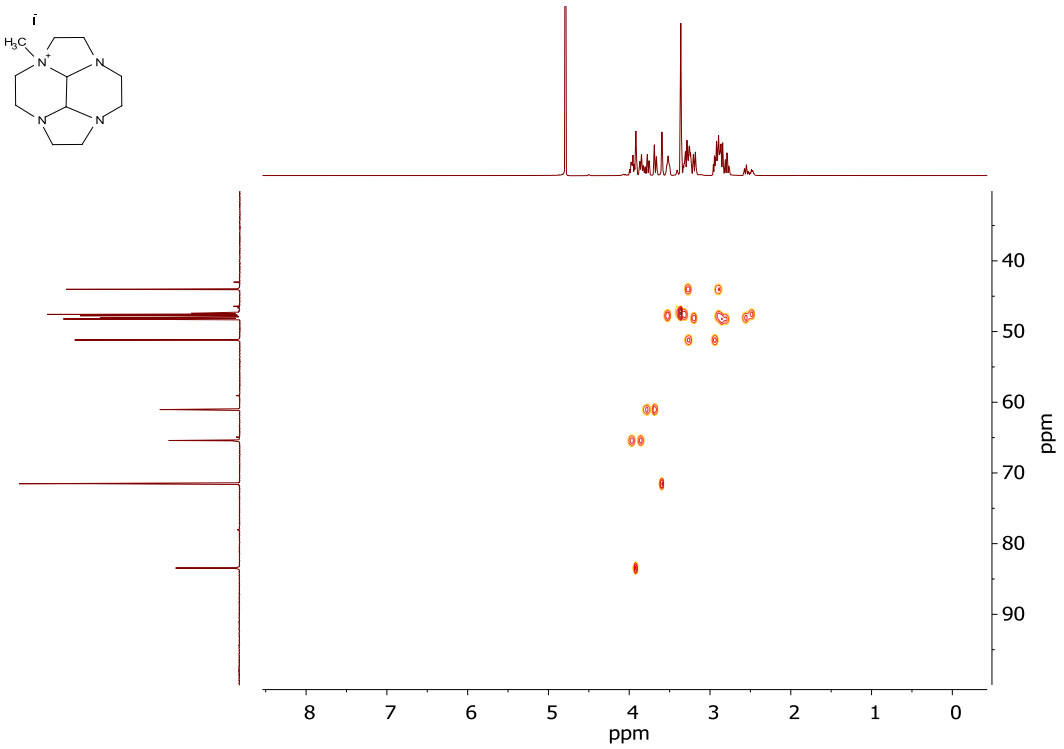
DEPT-RMN (D_2O) (δ/ppm)



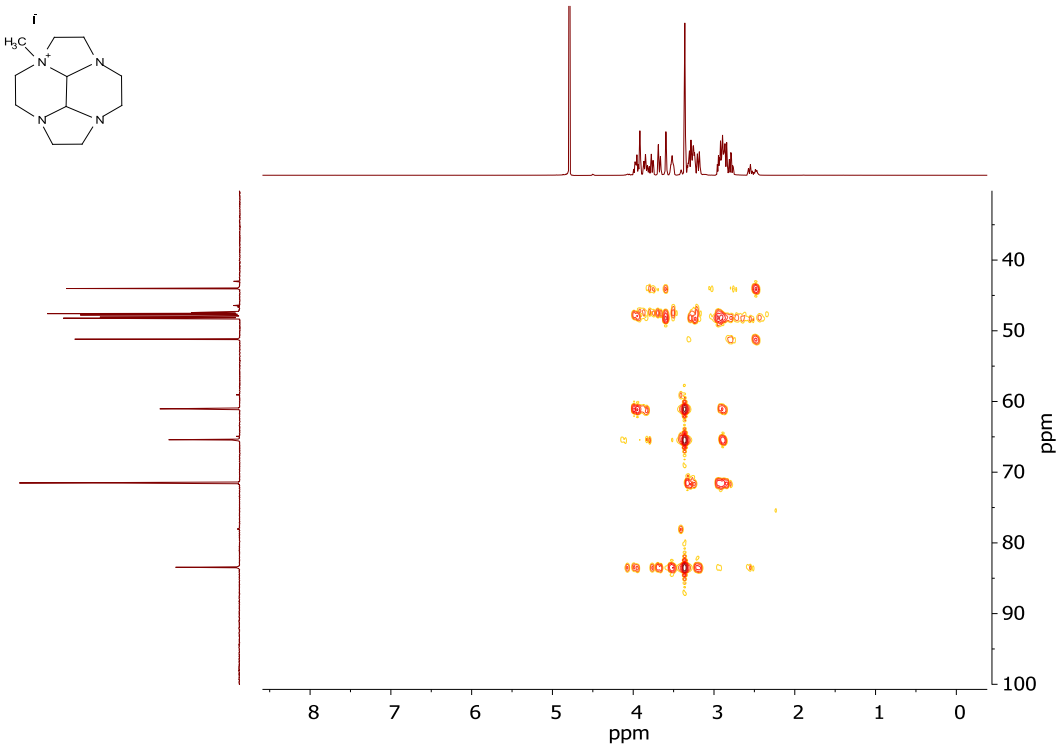
COSY-RMN (D_2O) (δ/ppm)



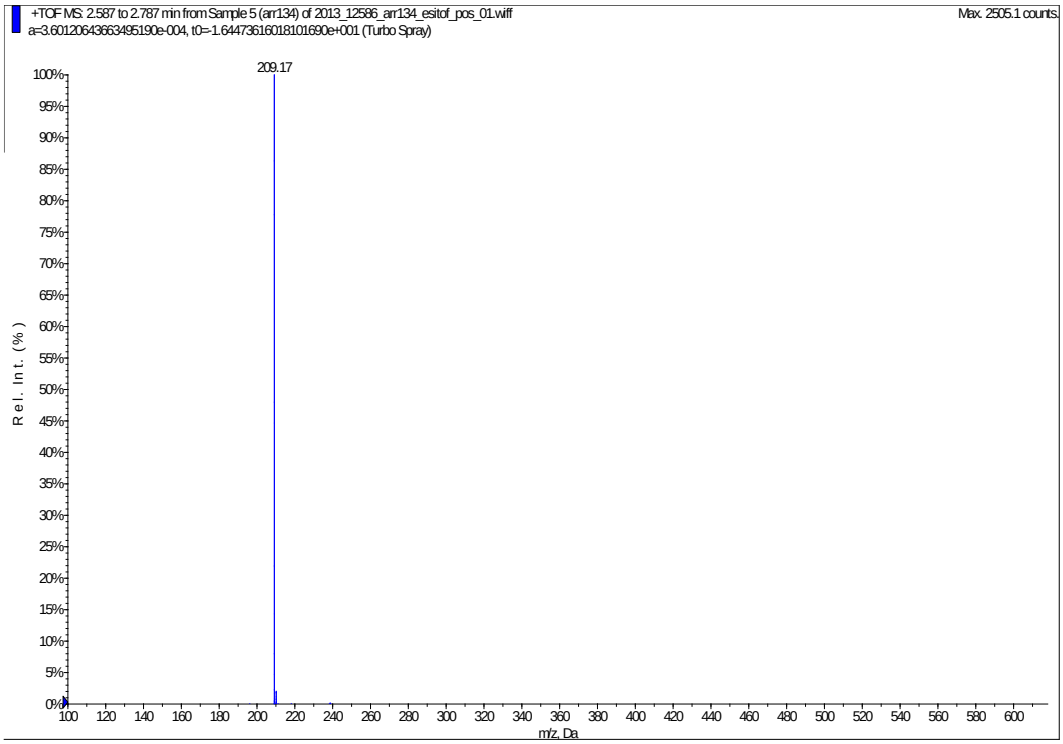
HSQC-RMN (D_2O) (δ/ppm)



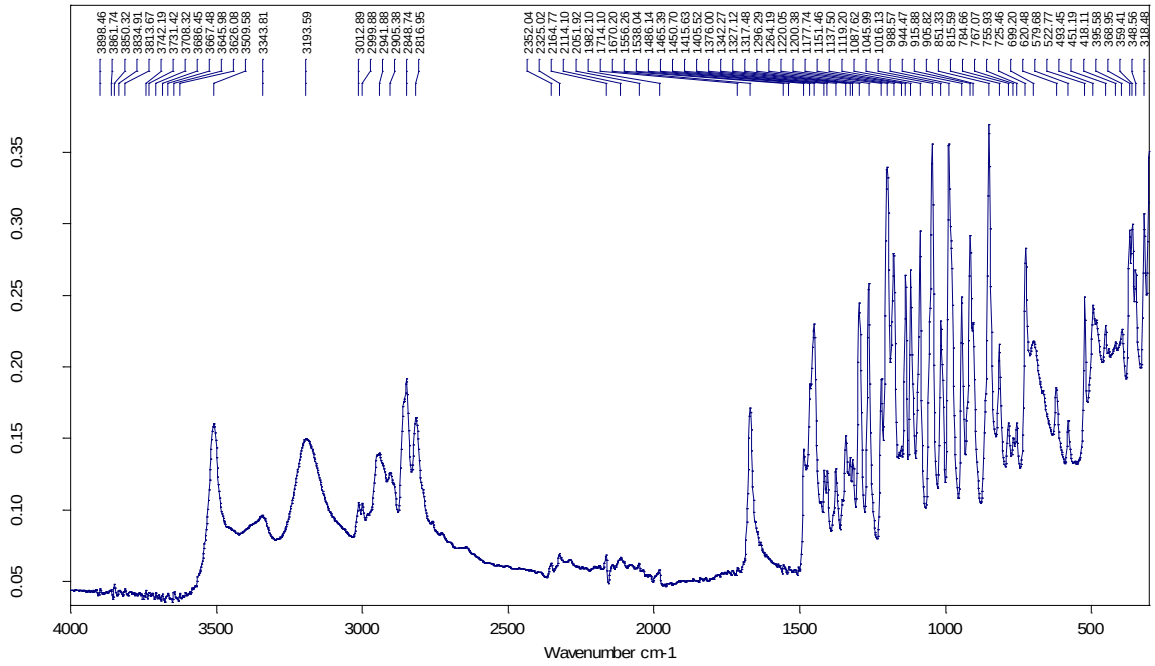
HMBC-RMN (D_2O) (δ/ppm)



Espectro de masas ESI+

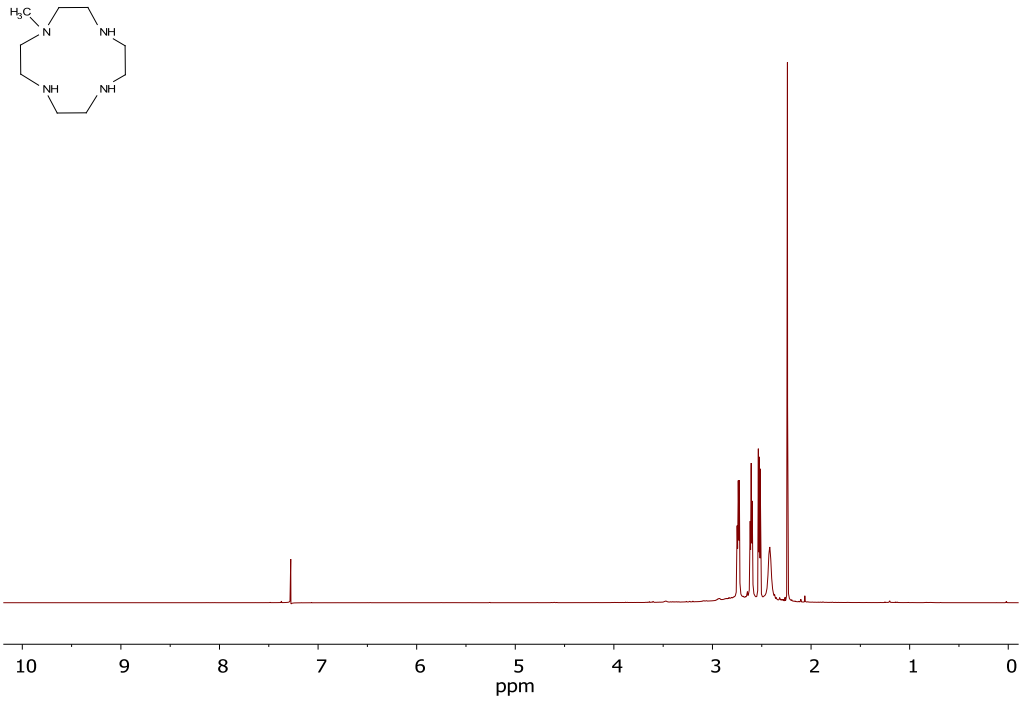


Espectro IR

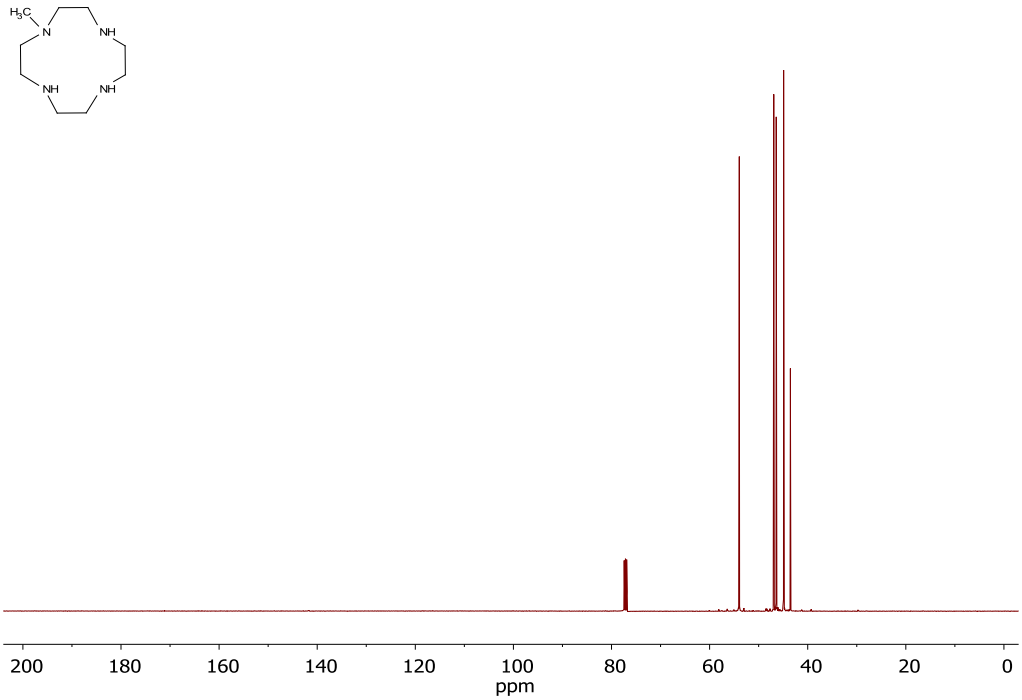


1 – Metil – 1,4,7,10 – tetraazaciclododecano (**12**)

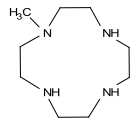
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)

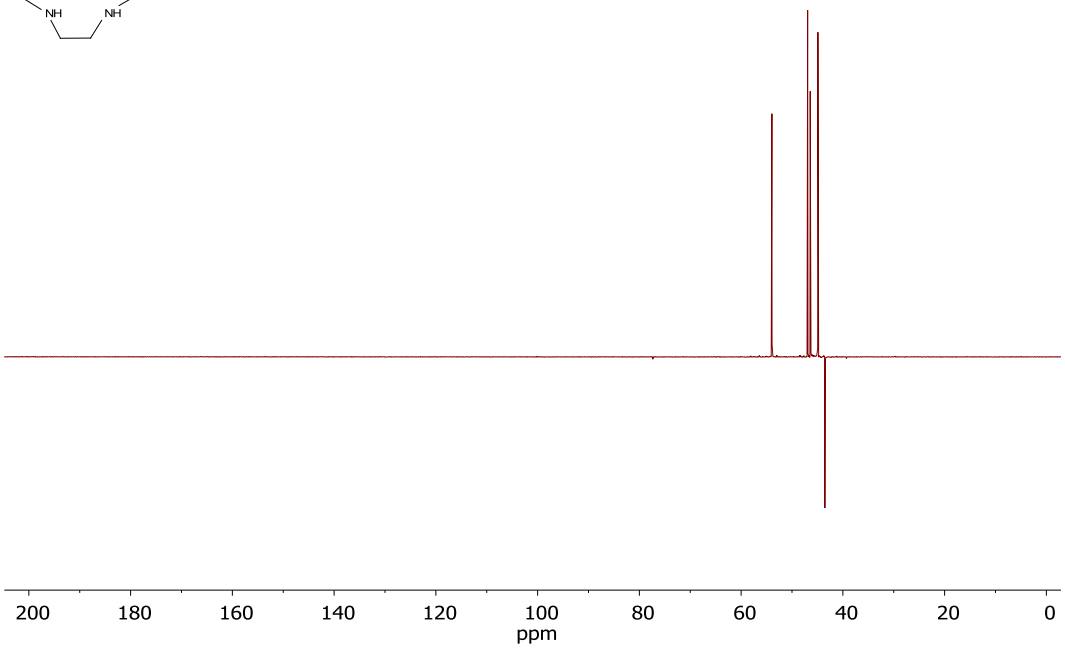


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

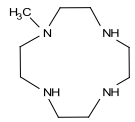


DEPT-RMN ($CDCl_3$) (δ/ppm)

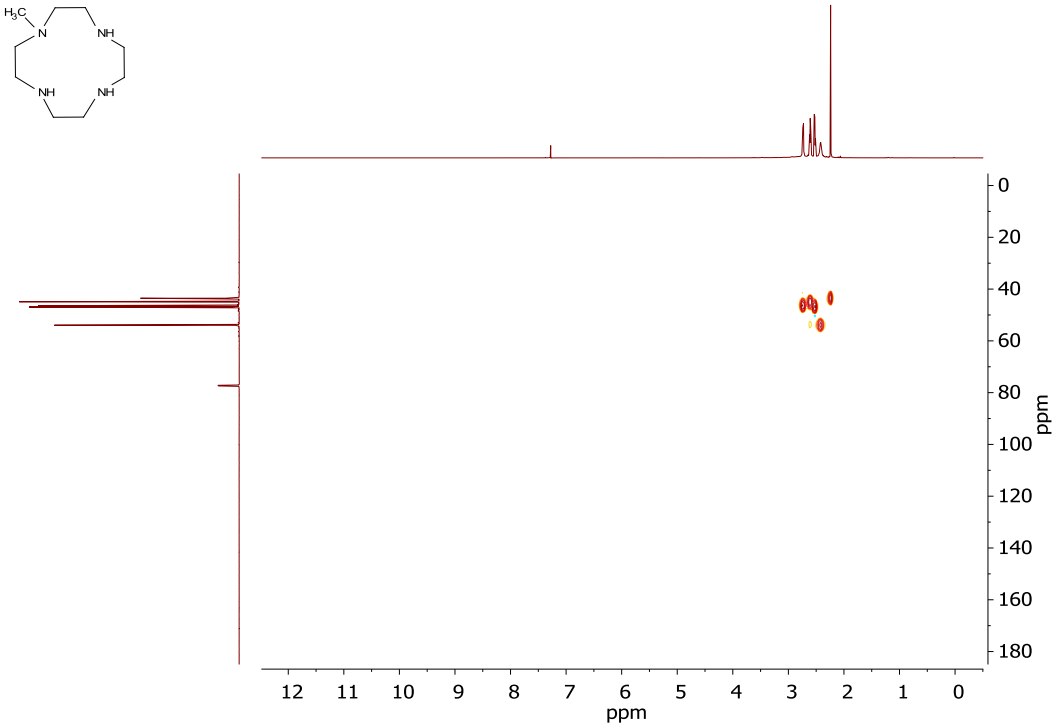




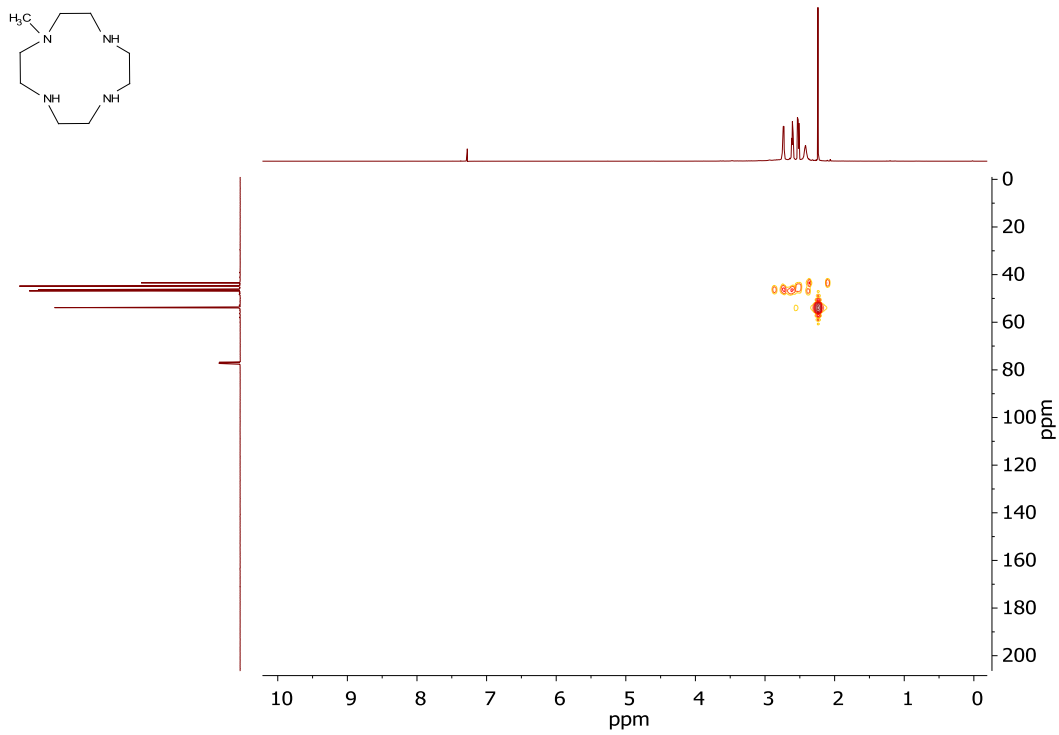
COSY-RMN ($CDCl_3$) (δ/ppm)



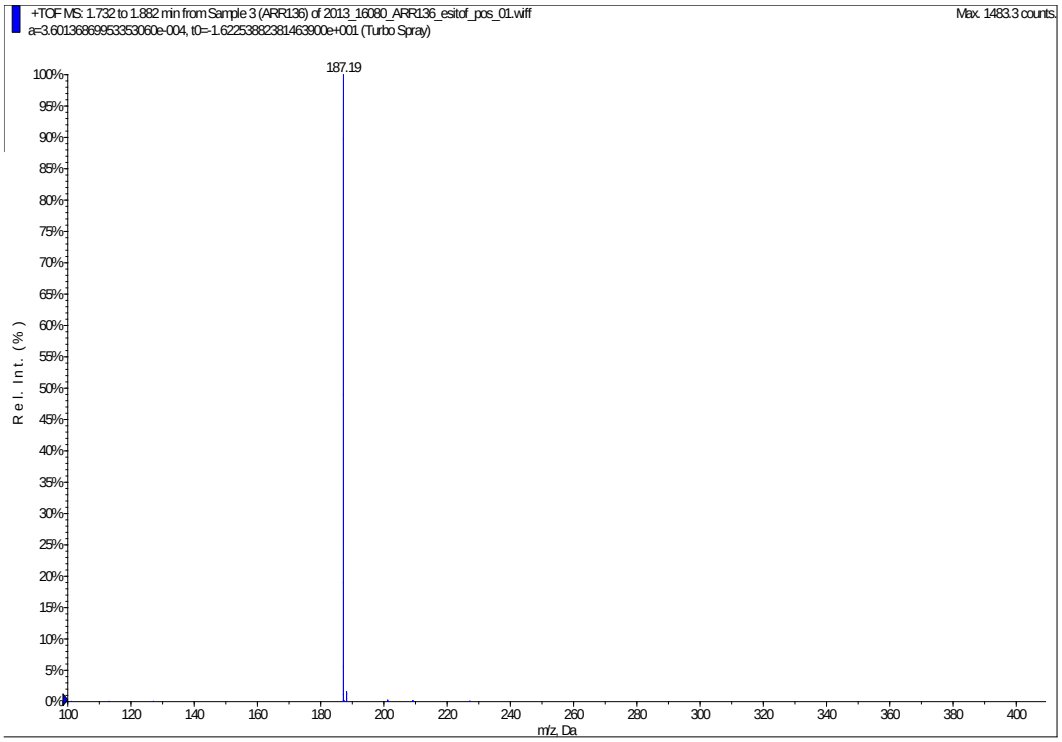
HSQC-RMN ($CDCl_3$) (δ/ppm)



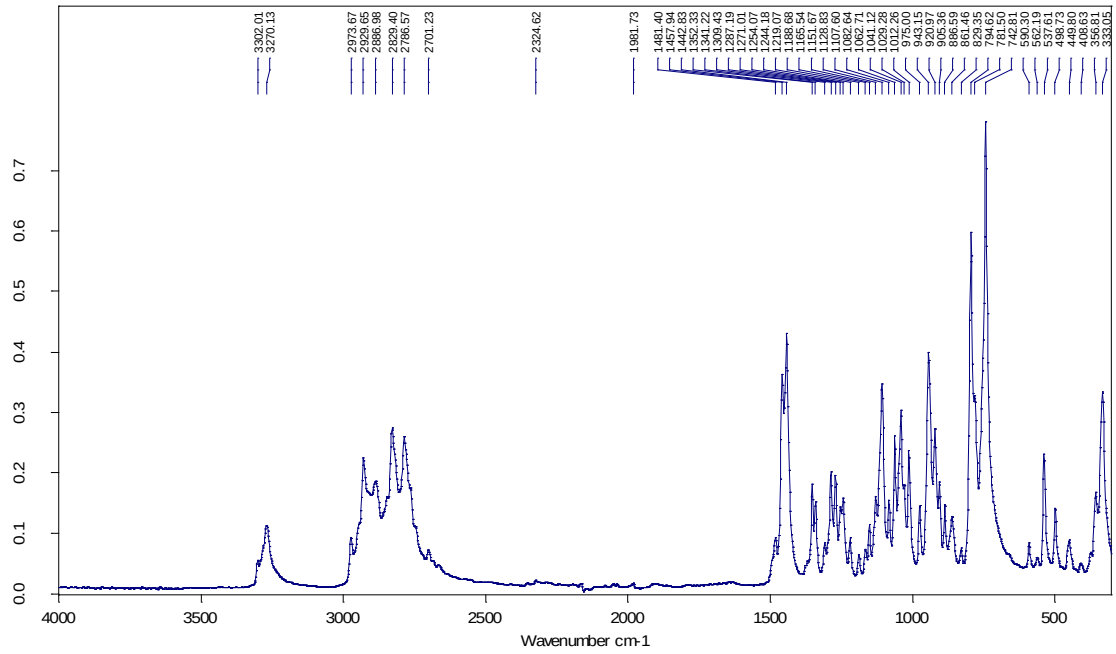
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

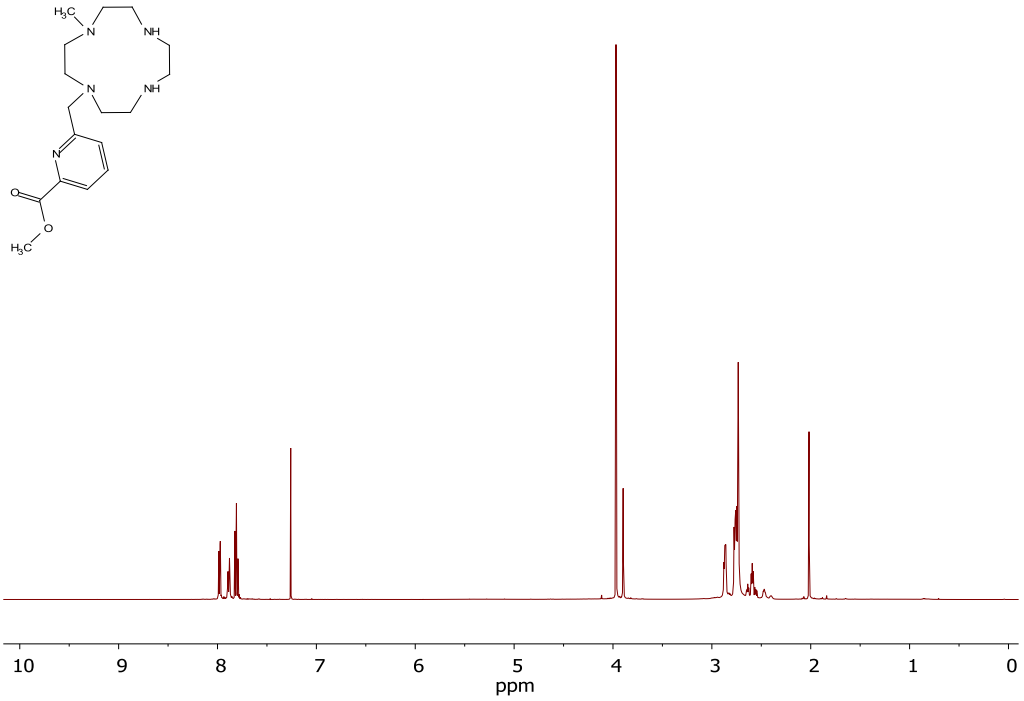


Espectro IR

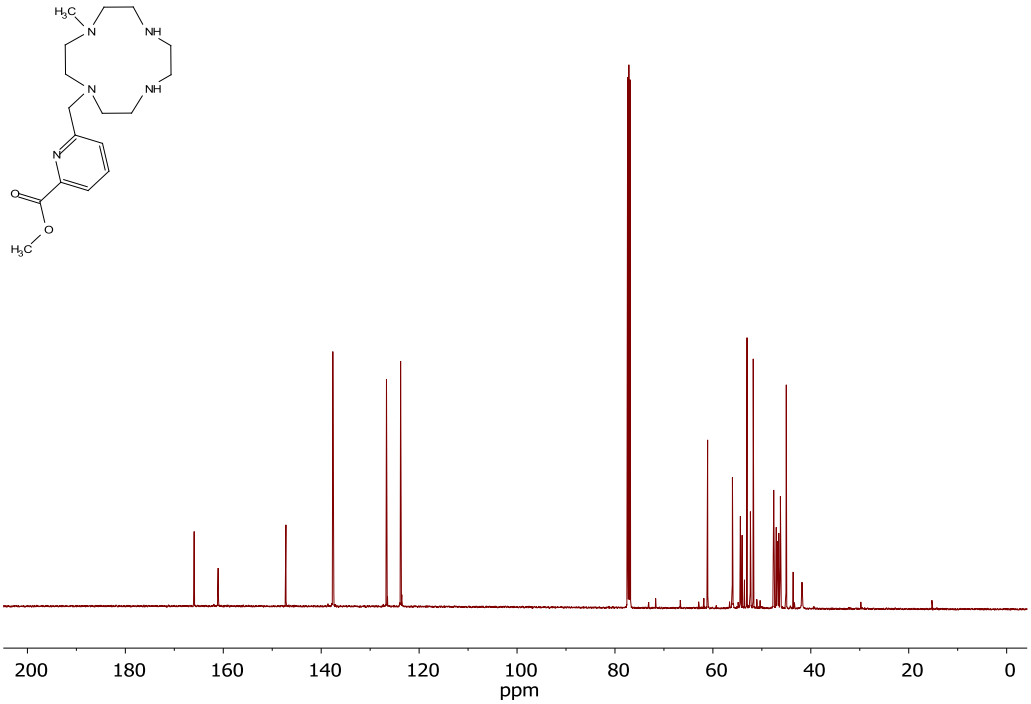


Metil 6 - ((4 – metil - 1,4,7,10 – tetraazaciclododecan – 1 - il)metil)picolinato (**13**)

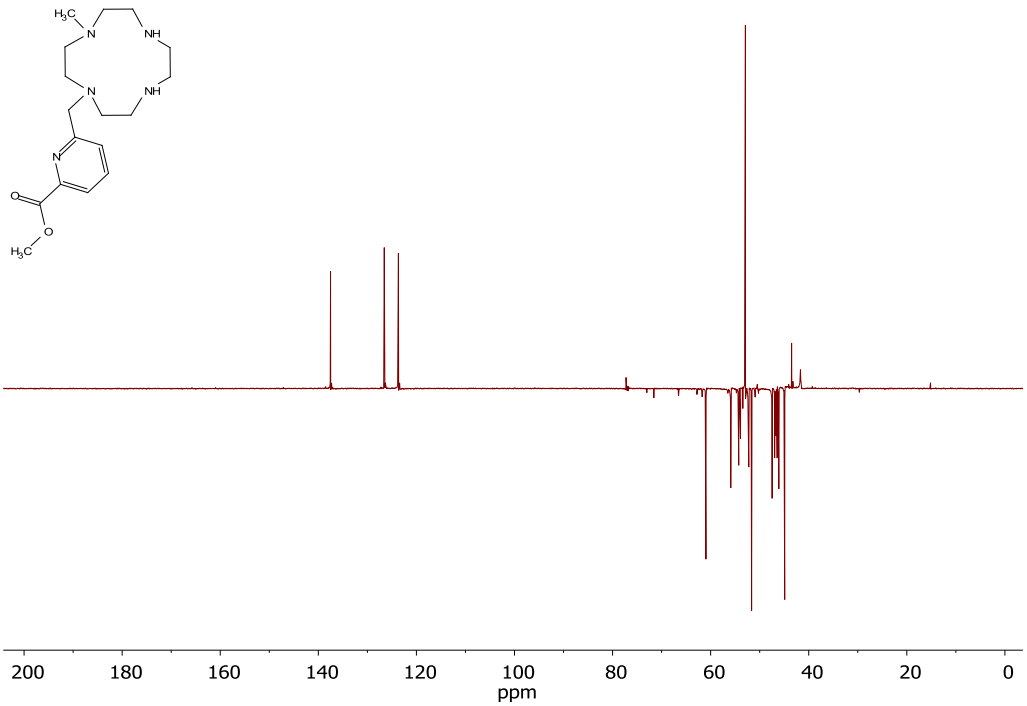
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



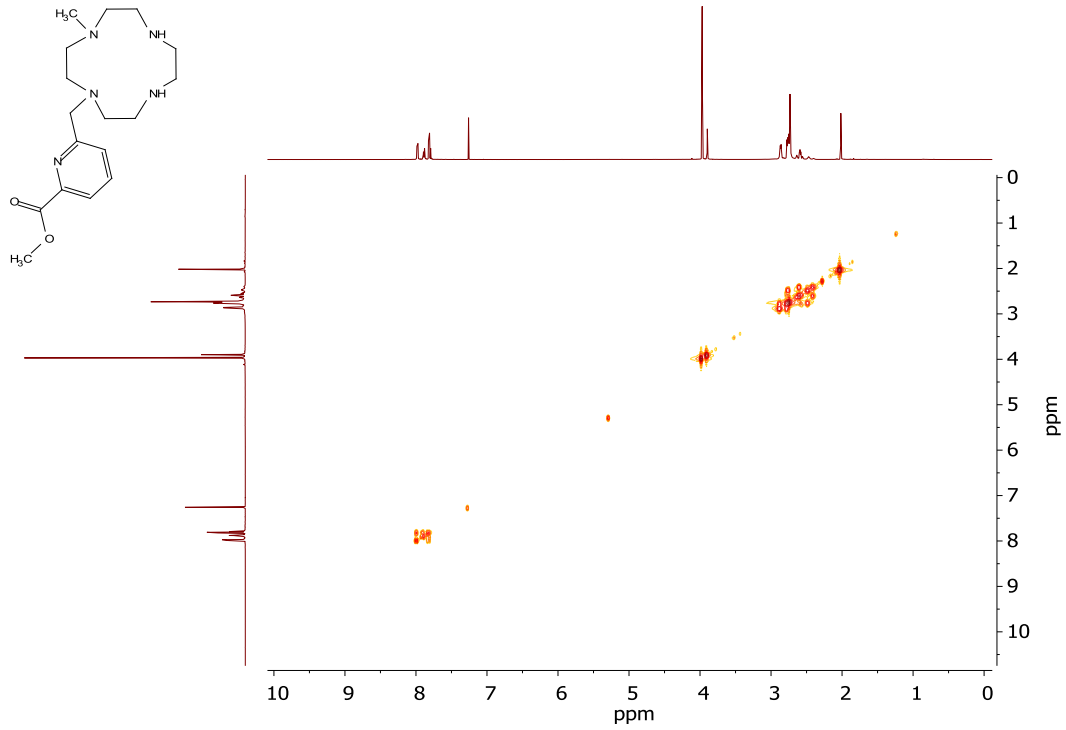
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



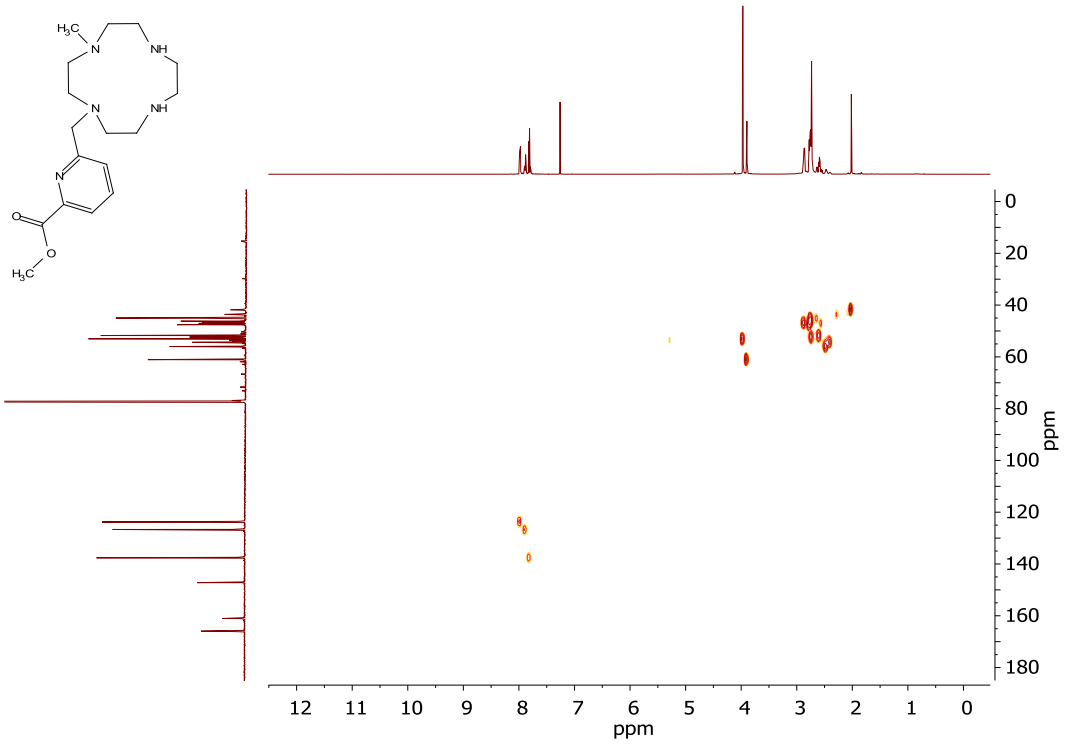
DEPT-RMN ($CDCl_3$) (δ/ppm)



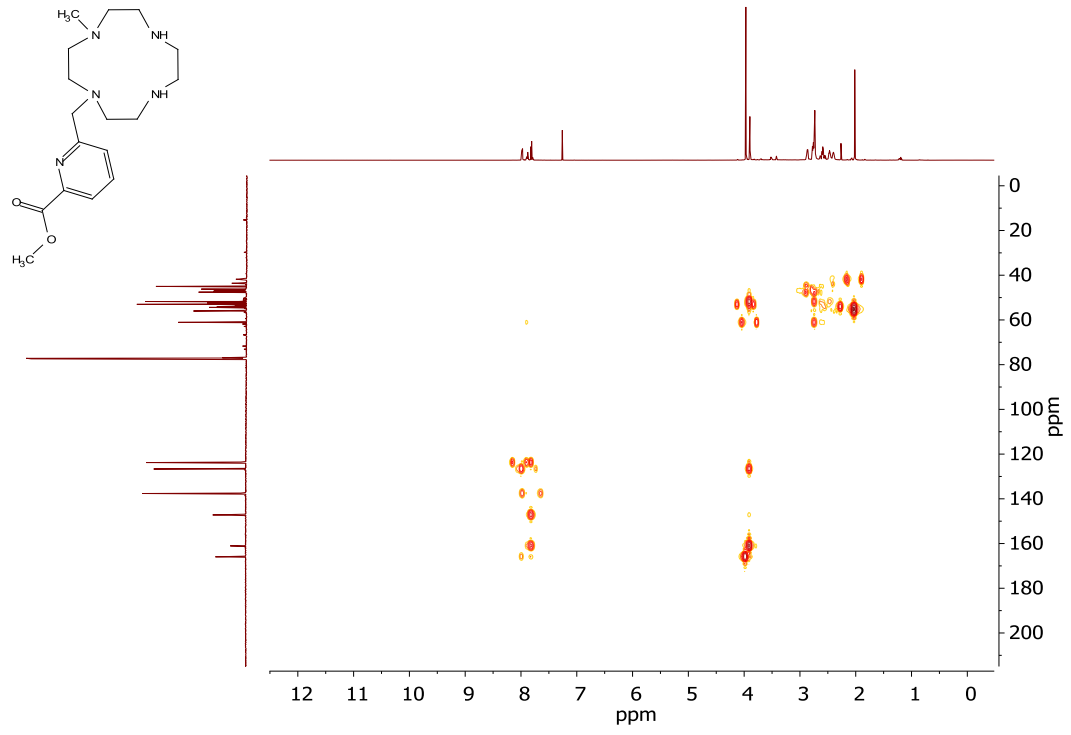
COSY-RMN ($CDCl_3$) (δ/ppm)



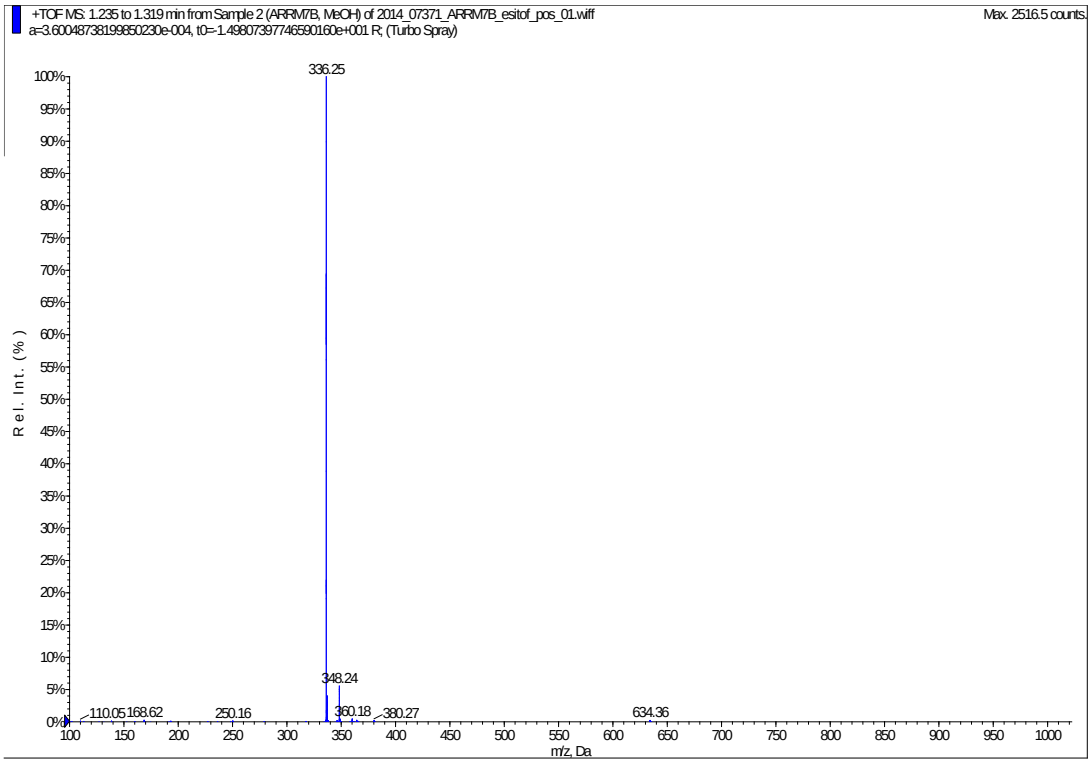
HSQC-RMN ($CDCl_3$) (δ/ppm)



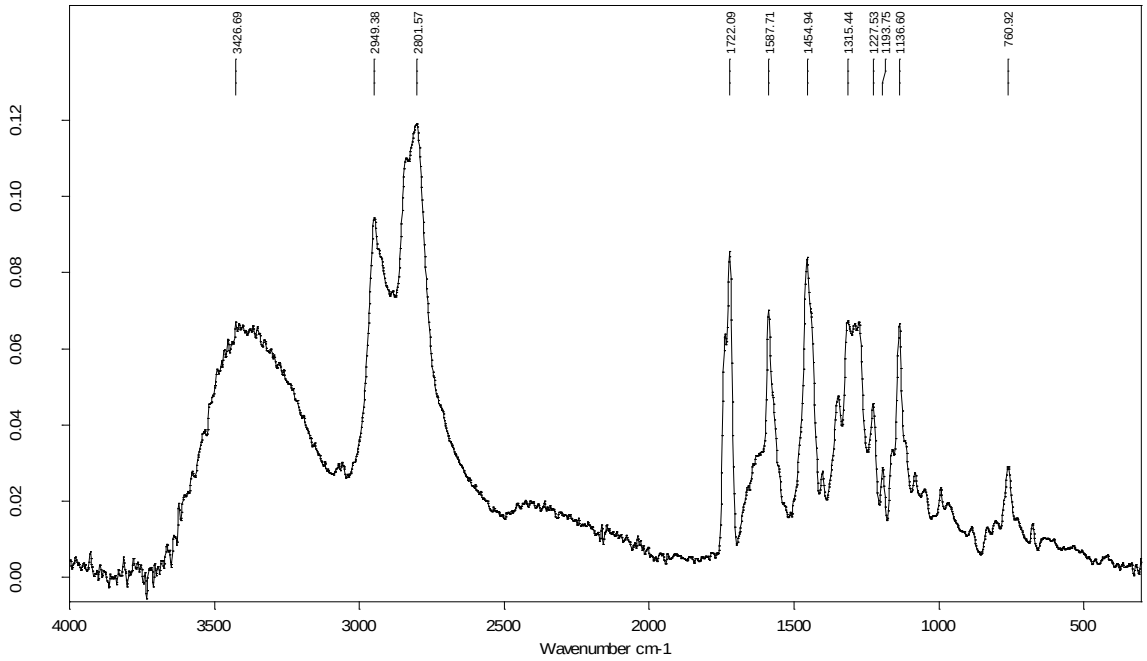
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

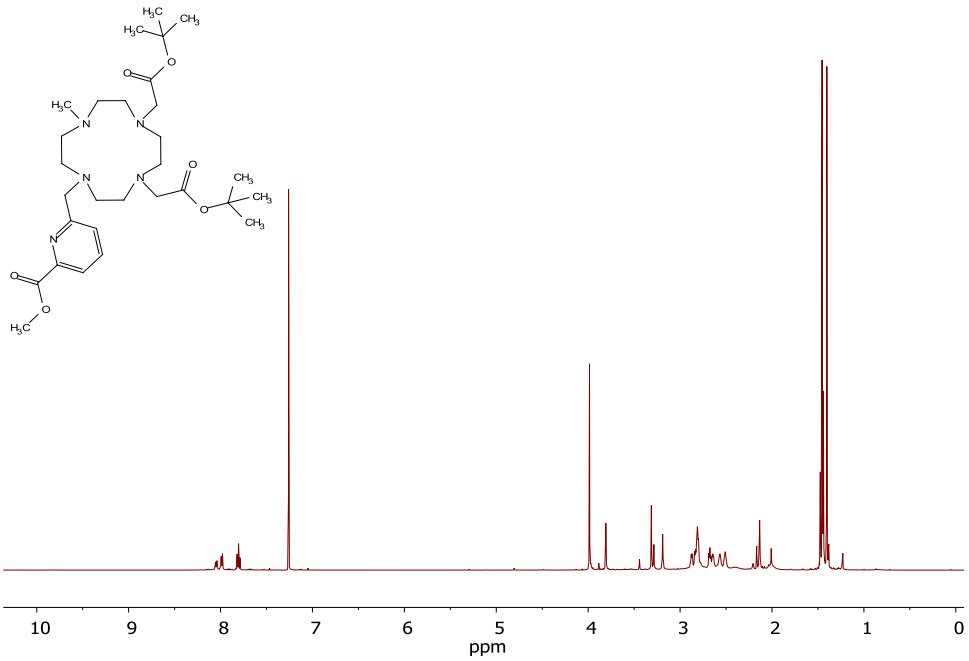


Espectro IR

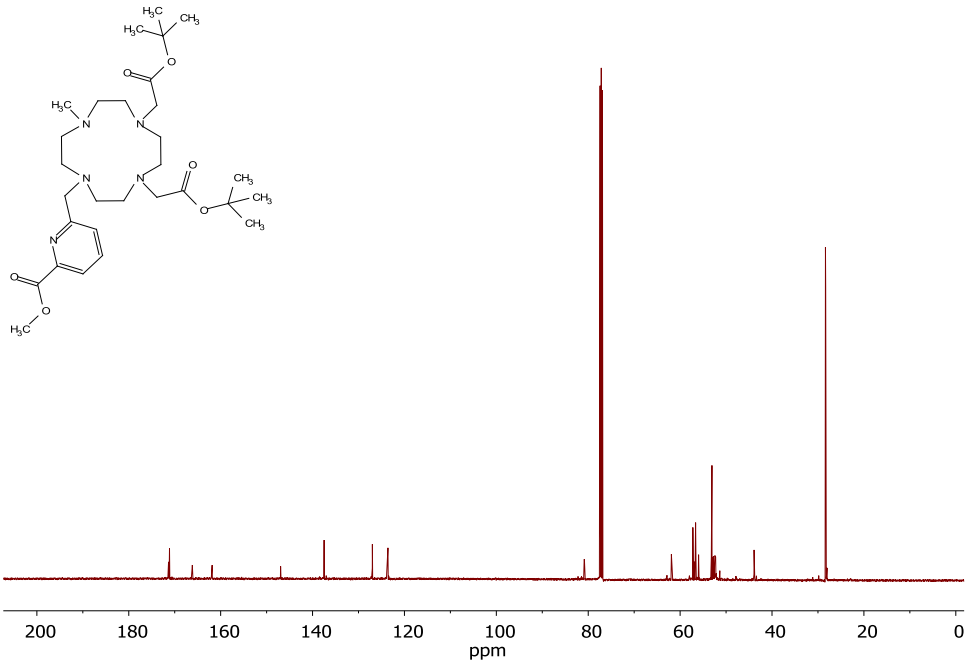


Diacetato de di-tert-butil 2,2' - (7 - ((6 - (metoxicarbonil)piridin – 2 - il)metil)-10-metil - 1,4,7,10 – tetraazaciclododecano - 1,4 - diil) (**14**)

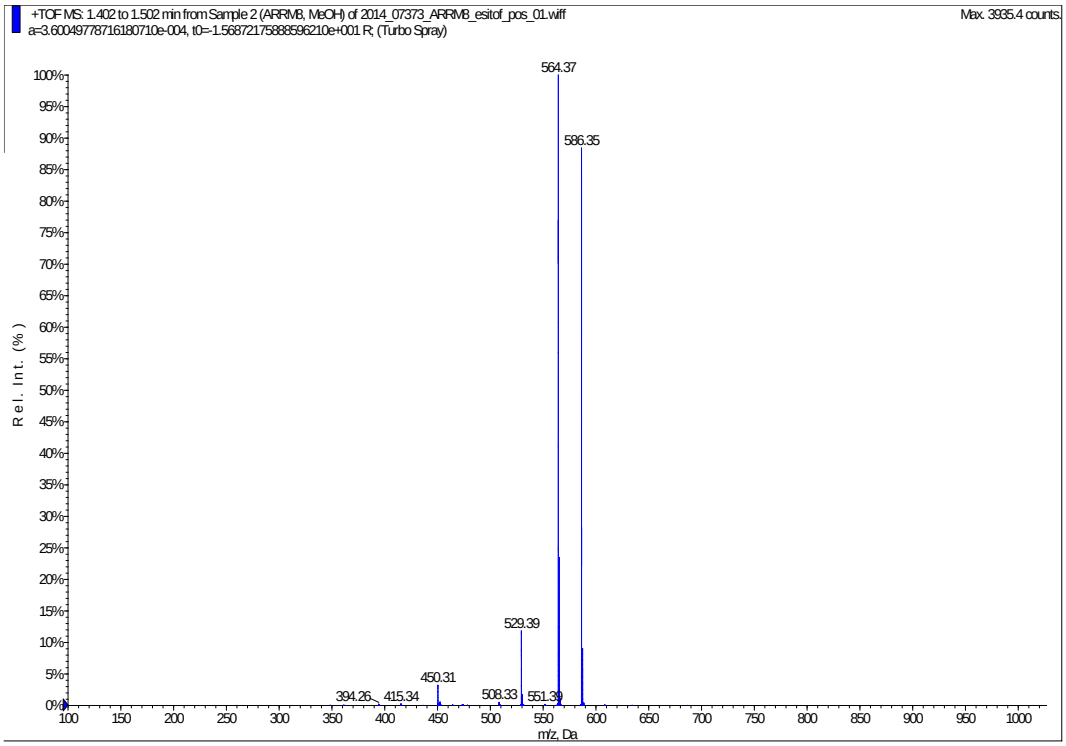
^{1}H-RMN ($CDCl_3$, 300 MHz) (δ/ppm)



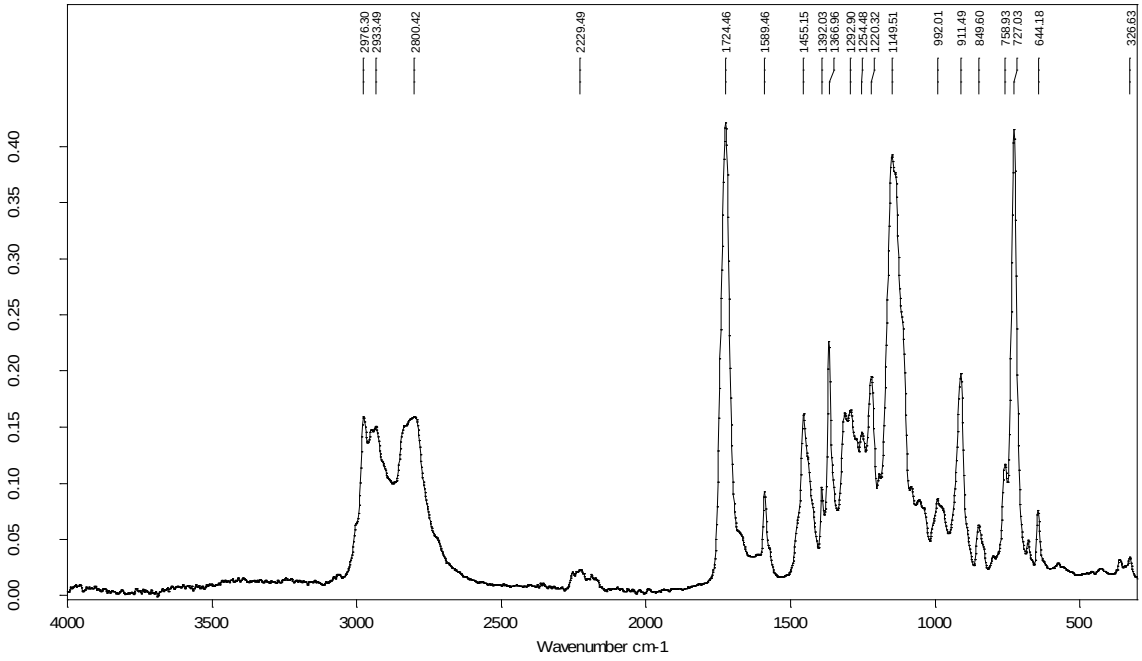
^{13}C-RMN ($CDCl_3$, 75,5 MHz) (δ/ppm)



Espectro de masas ESI+

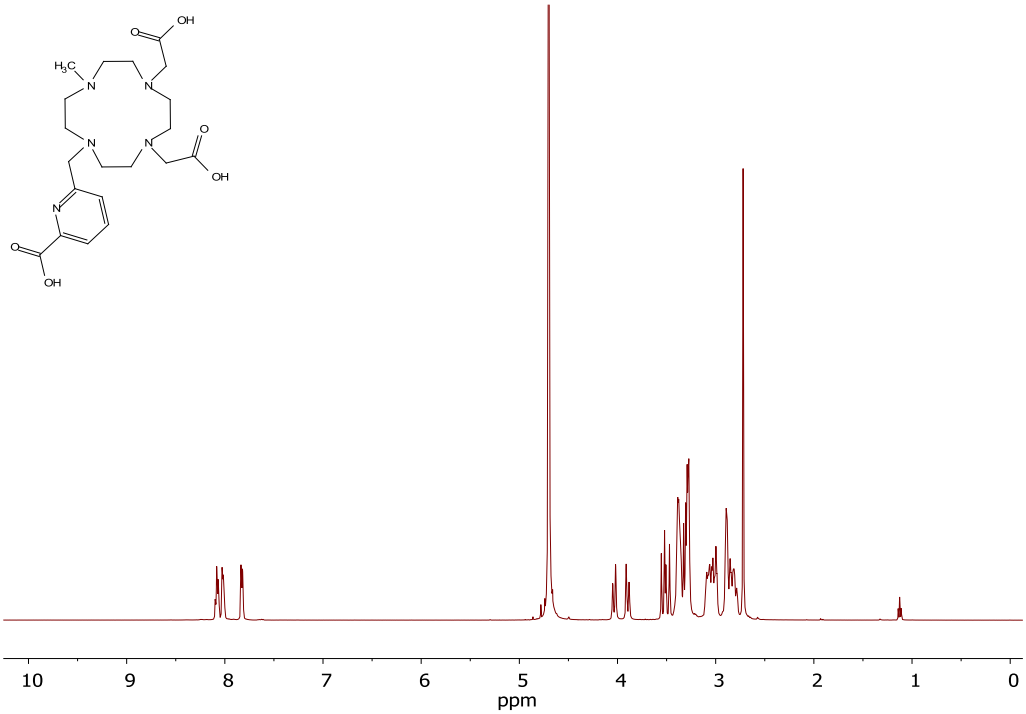


Espectro IR

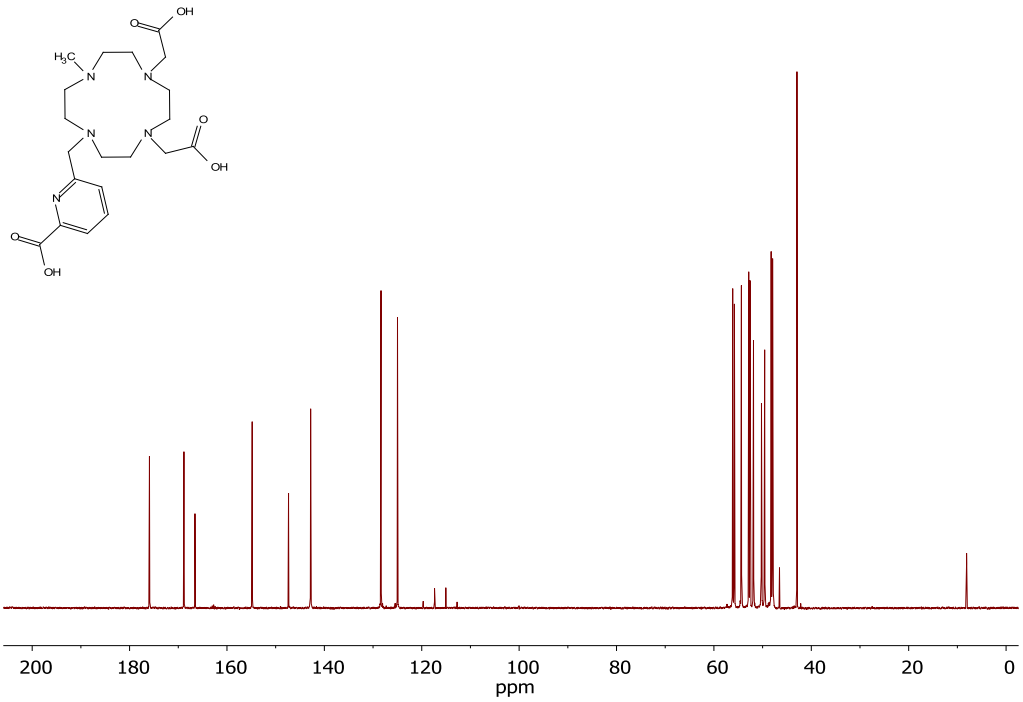


Ácido 2, 2´ - (7 – ((6 –carboxipiridin – 2 il)metil) – 10 – metil - 1, 4, 7, 10 – tetraazaciclododecano – 1, 4 – diil) diacético (**1,4-H_3Medo2apa·5HCl·2H_2O**)

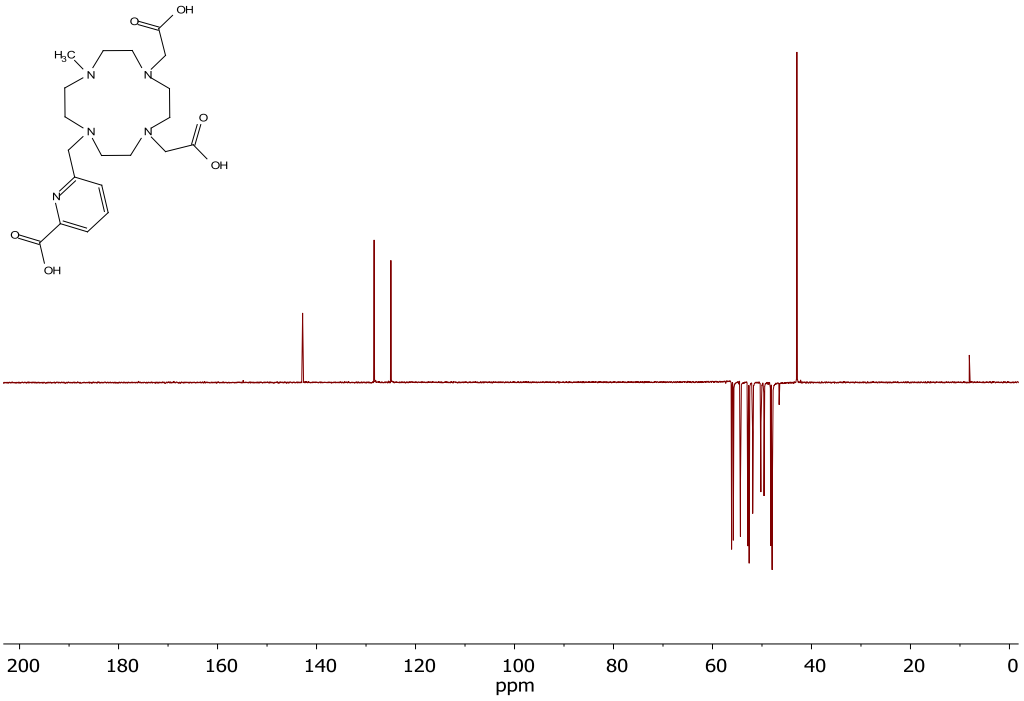
^{1}H-RMN (D_2O, 500 MHz, pD ~ 7) (δ/ppm)



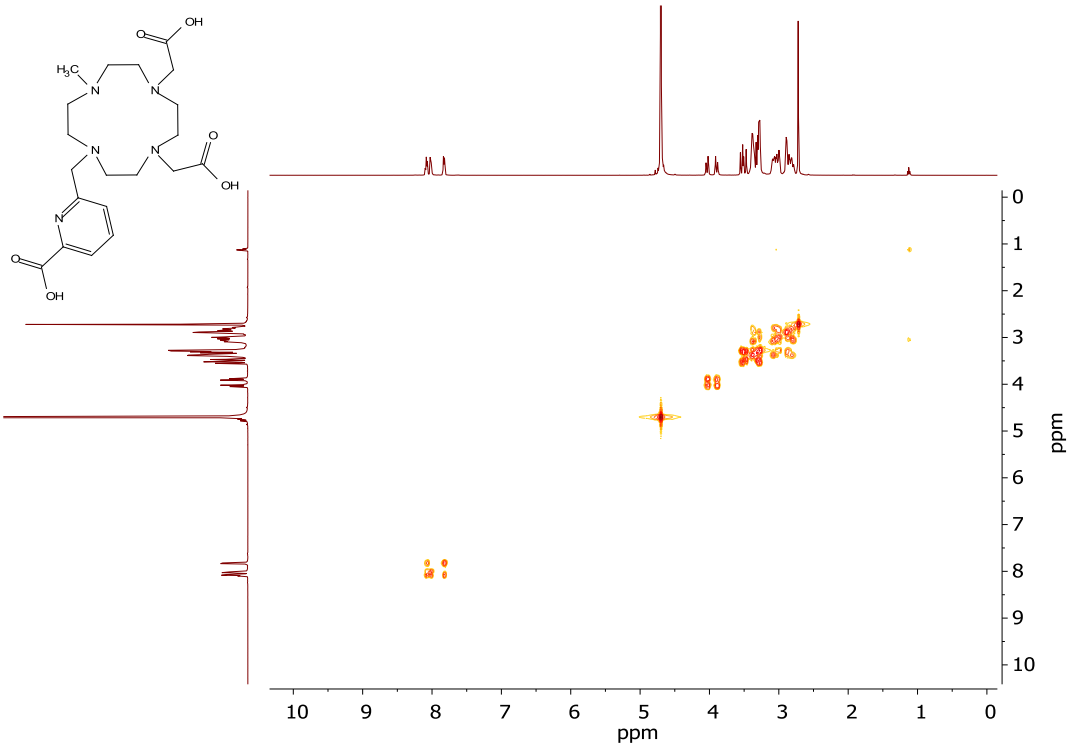
^{13}C-RMN (D_2O, 125,8 MHz, pD ~ 7) (δ/ppm)



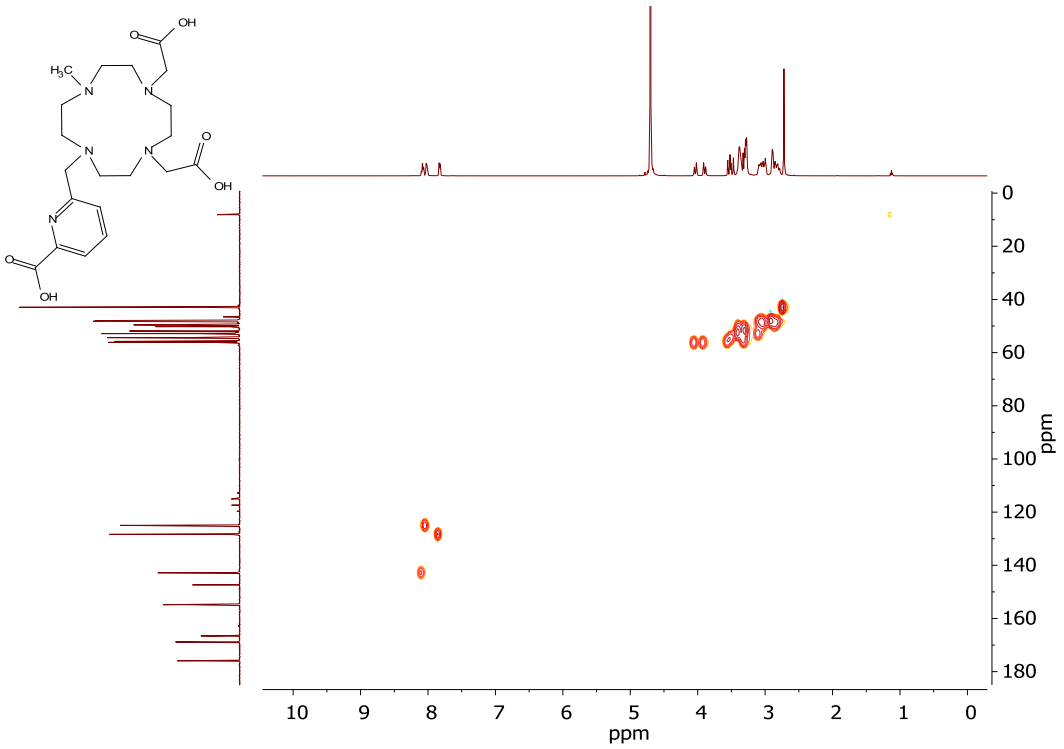
DEPT-RMN (D_2O, pD ~ 7) (δ/ppm)



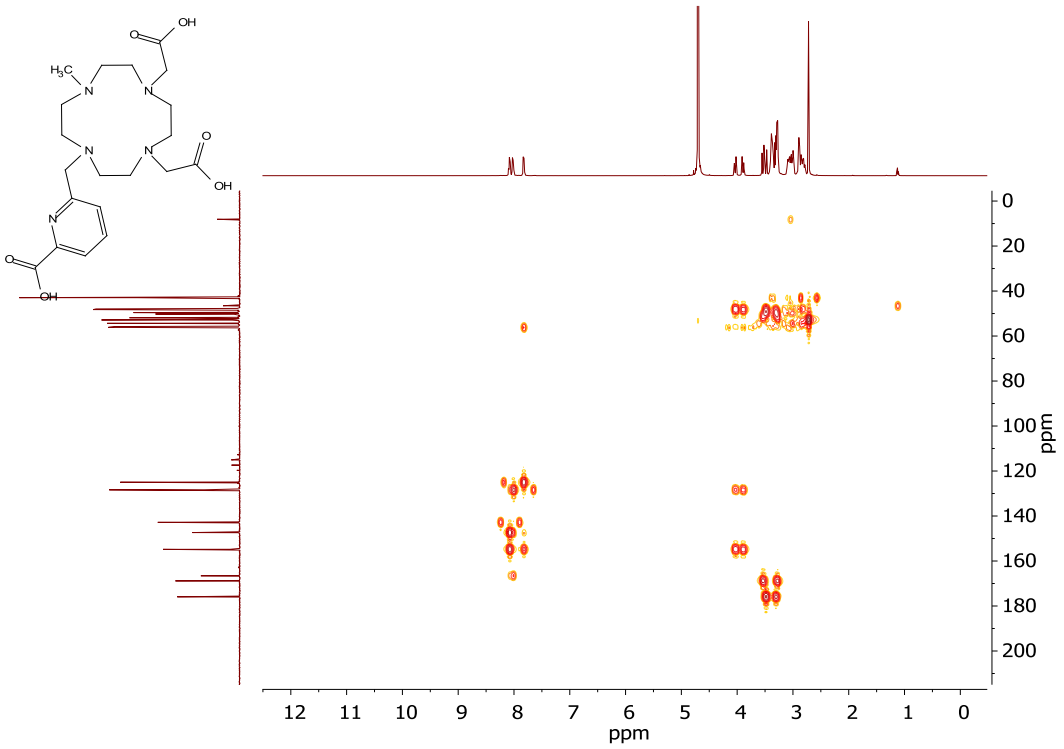
COSY-RMN (D_2O, pD ~ 7) (δ/ppm)



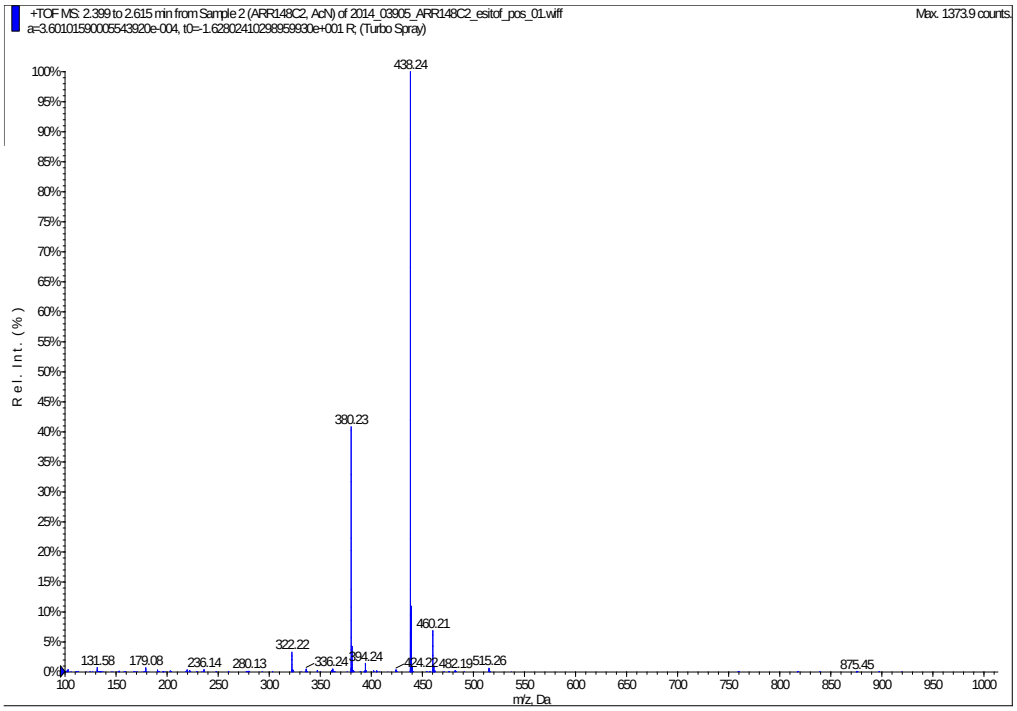
HSQC-RMN (D_2O, pD ~ 7) (δ/ppm)



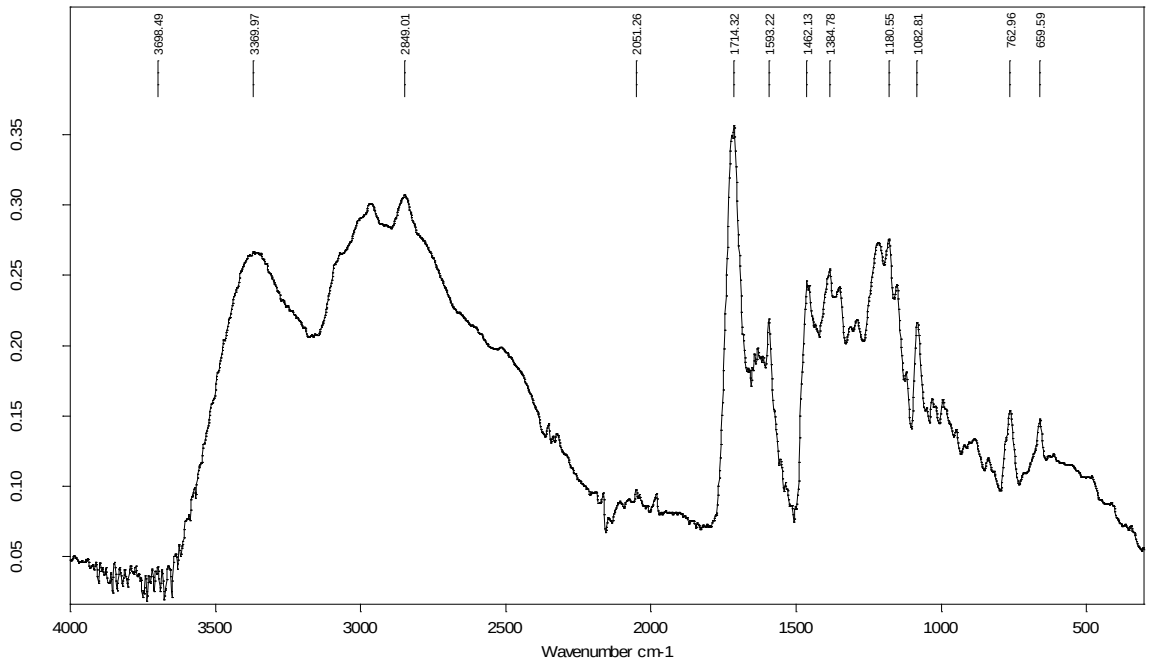
HMBC-RMN (D_2O, pD ~ 7) (δ/ppm)



Espectro de masas ESI+

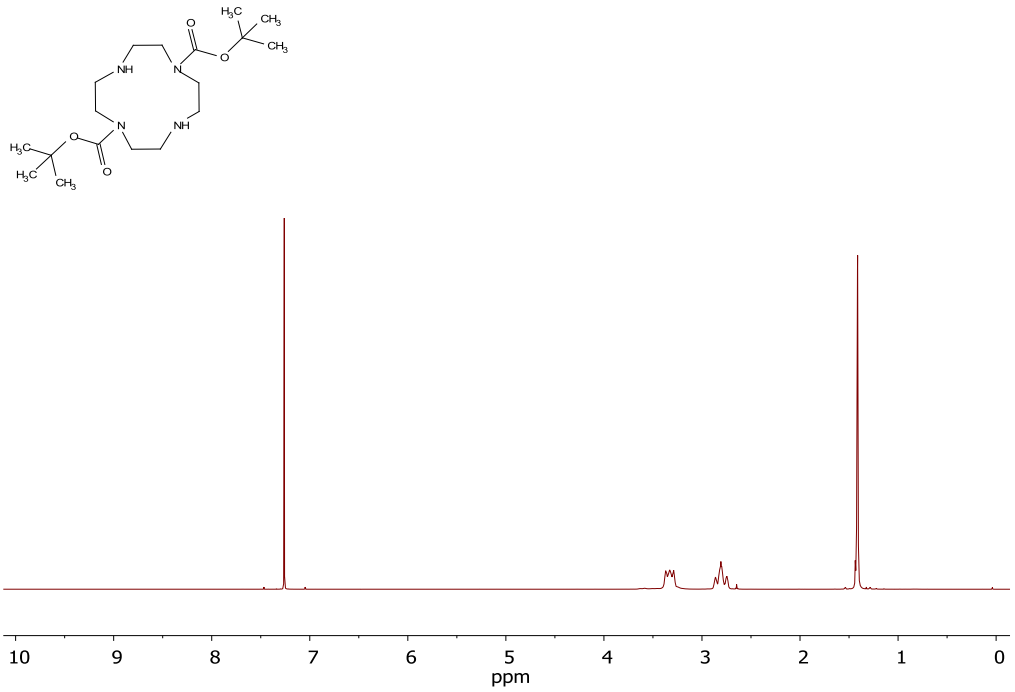


Espectro IR

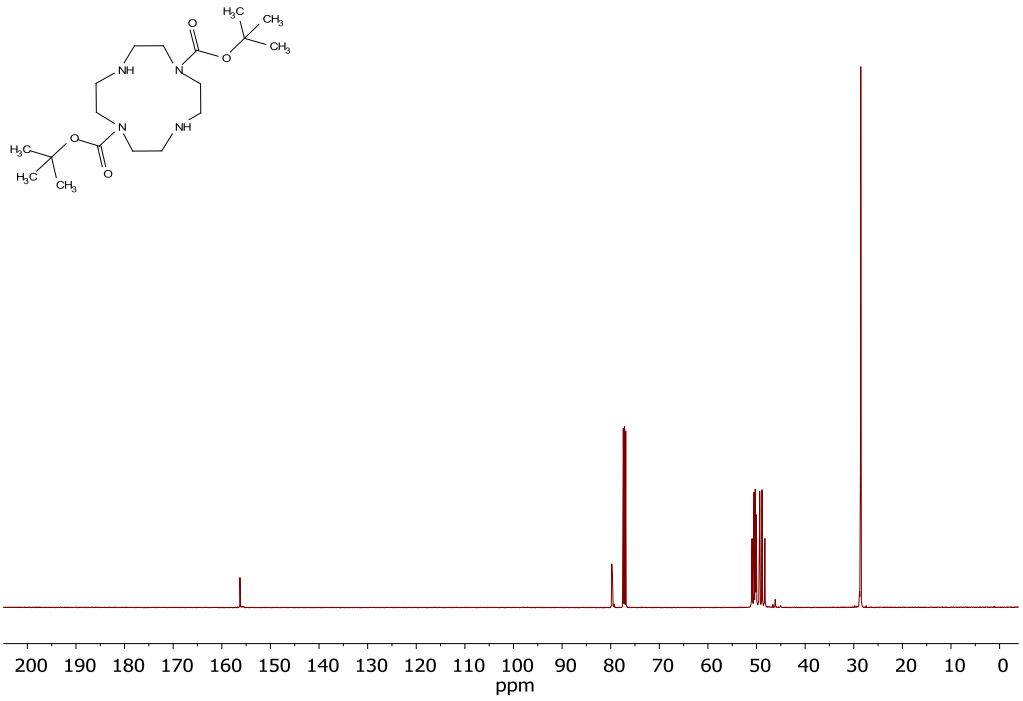


Di – *tert* - butil 1,4,7,10 – tetraazaciclododecano - 1,7 - dicarboxilato (**15**)

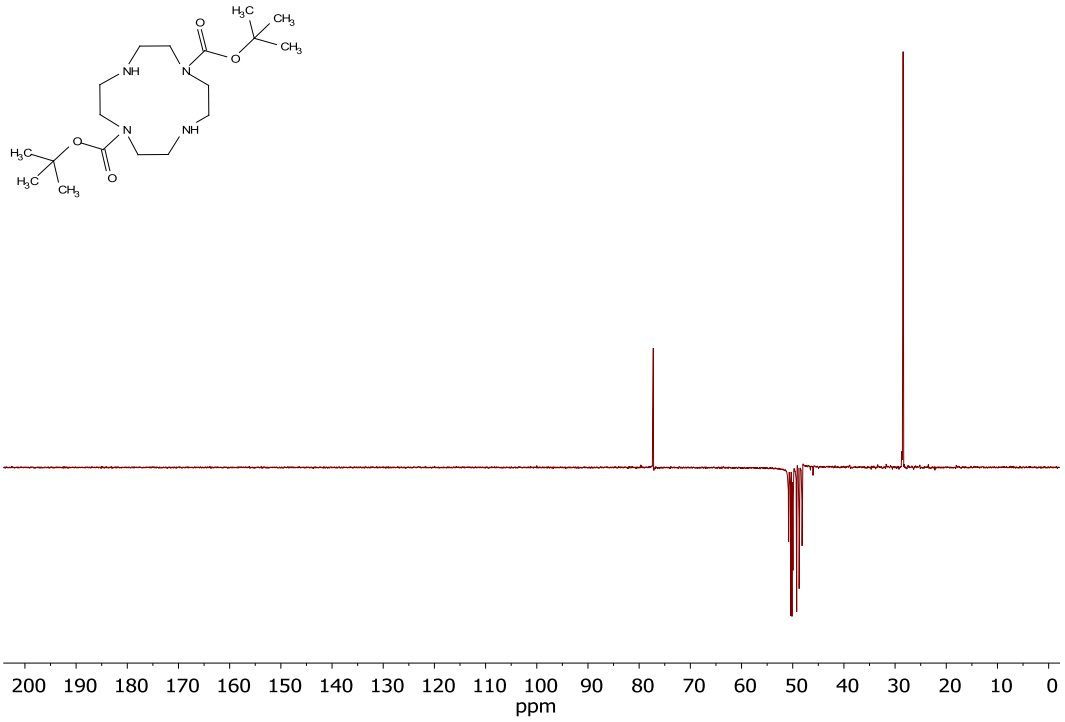
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



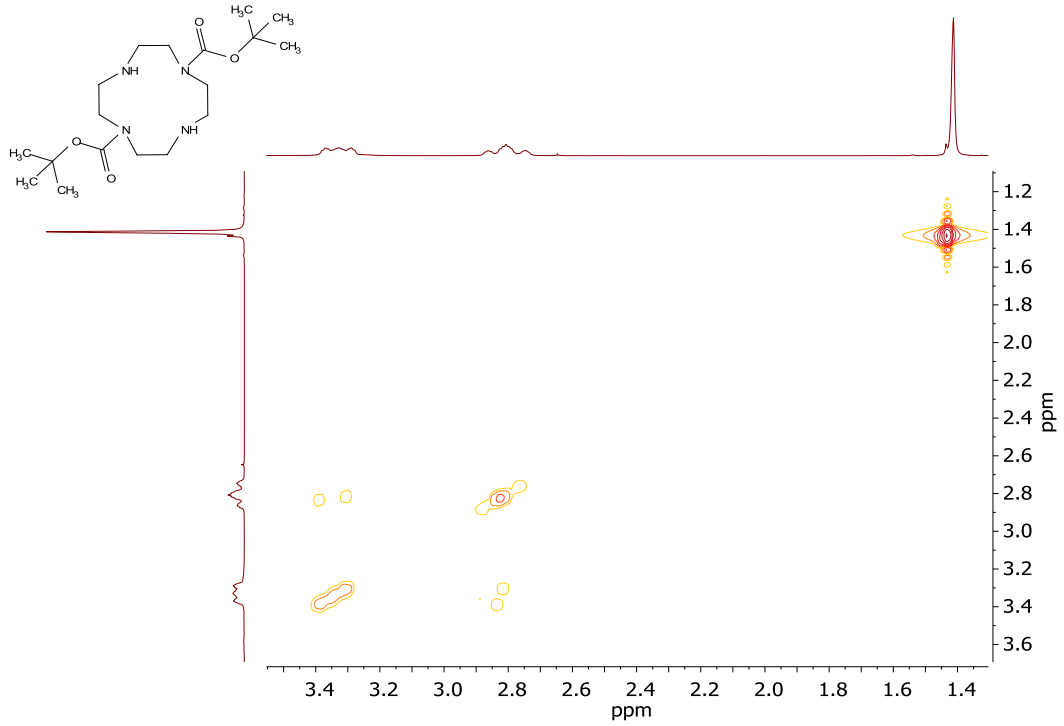
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



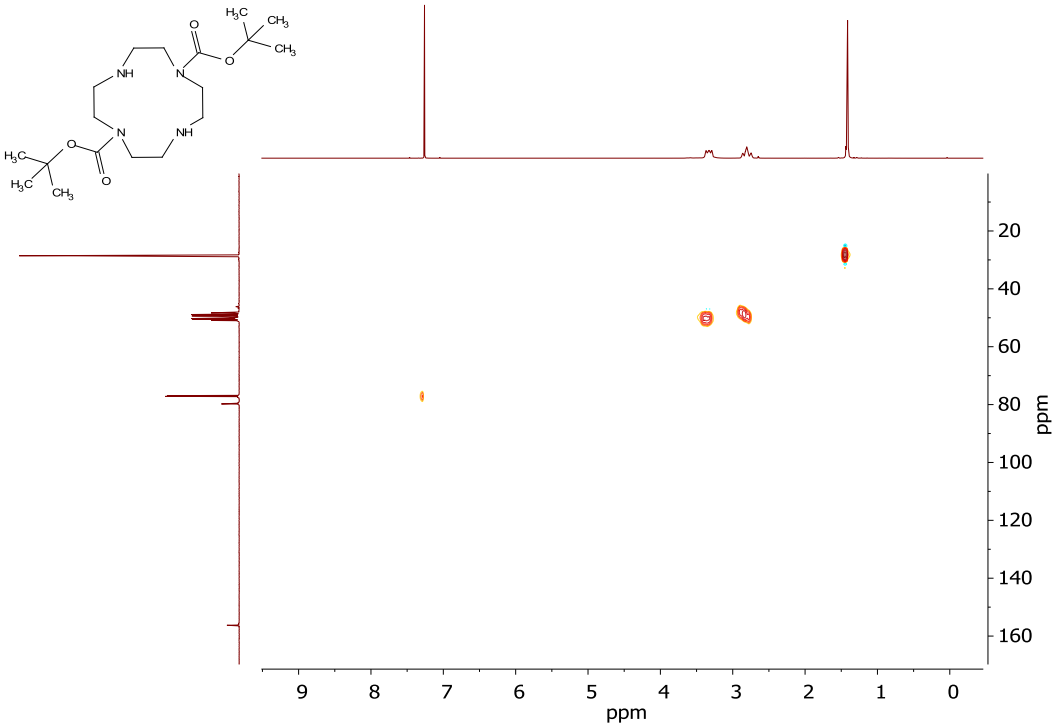
DEPT-RMN ($CDCl_3$) (δ/ppm)



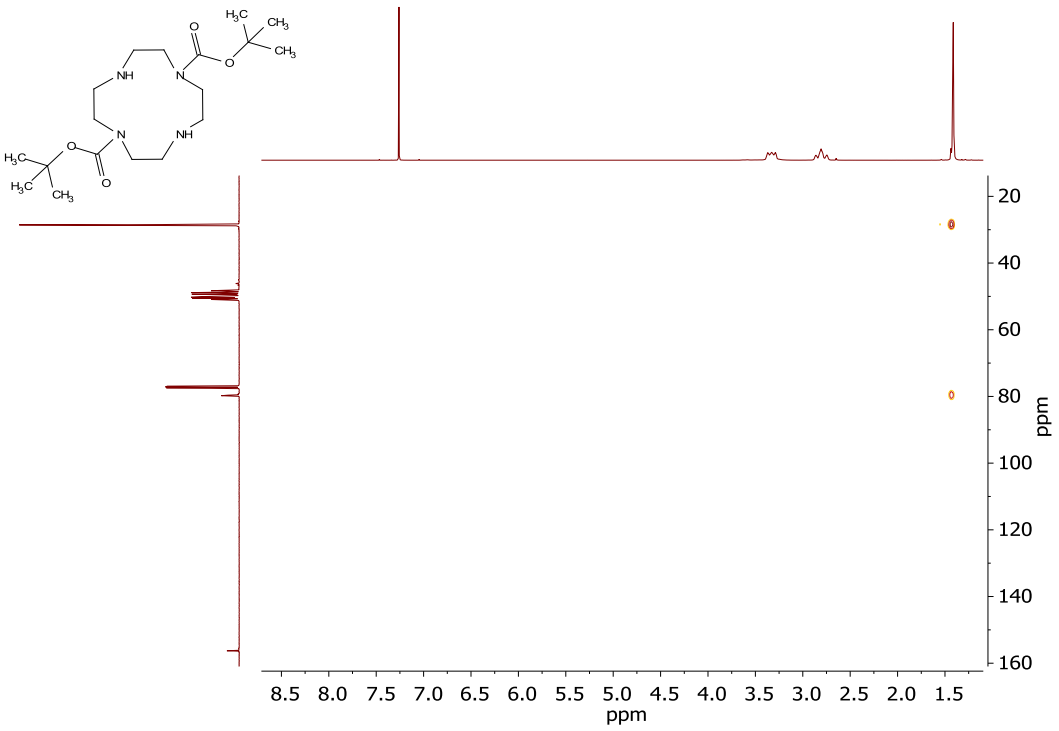
COSY-RMN ($CDCl_3$) (δ/ppm)



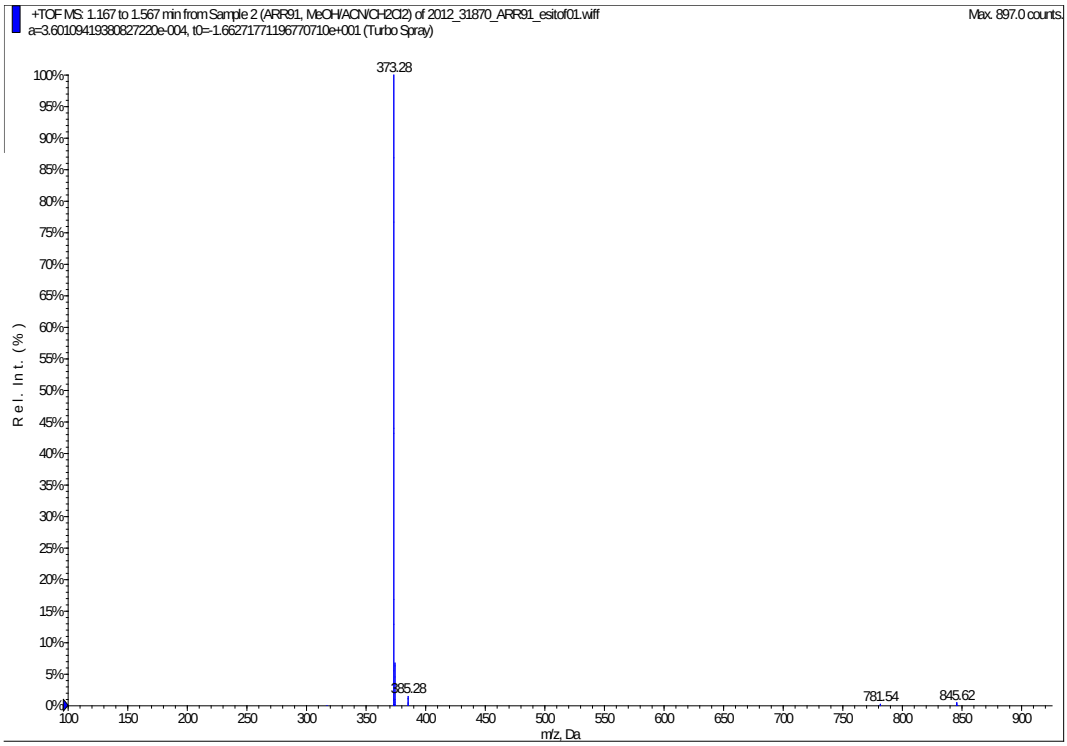
HSQC-RMN ($CDCl_3$) (δ/ppm)



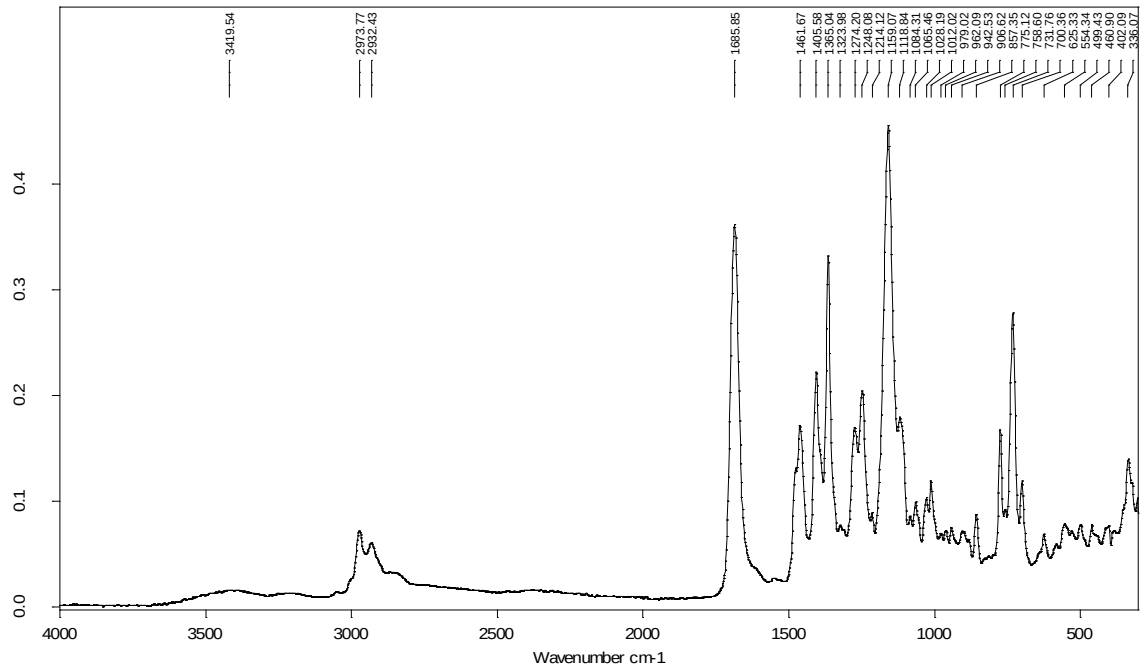
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

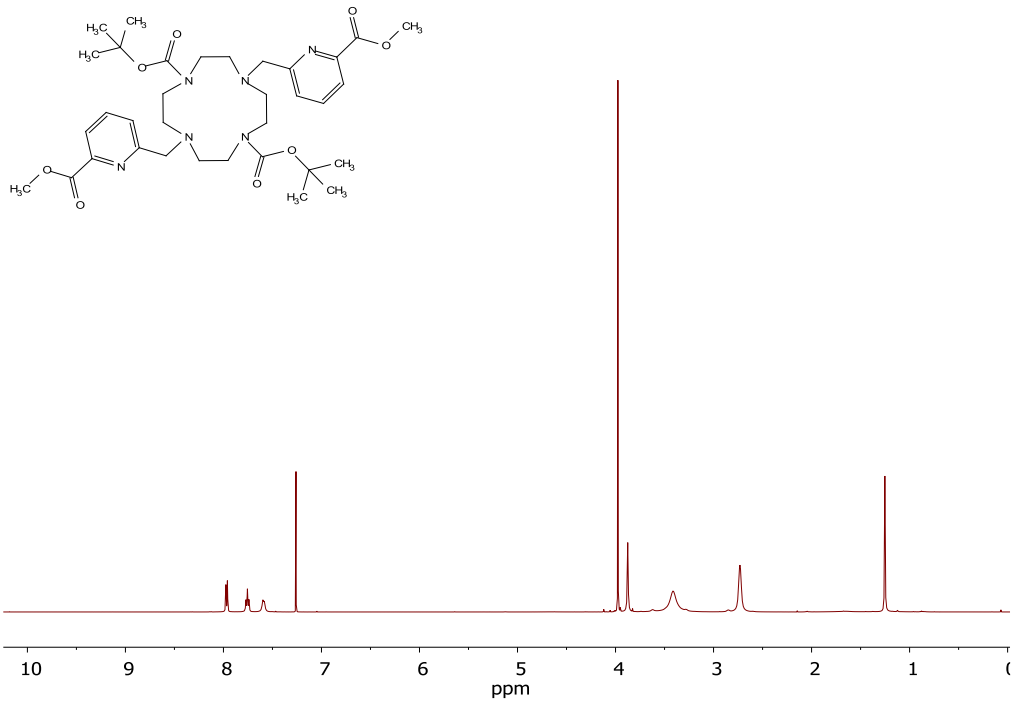


Espectro IR

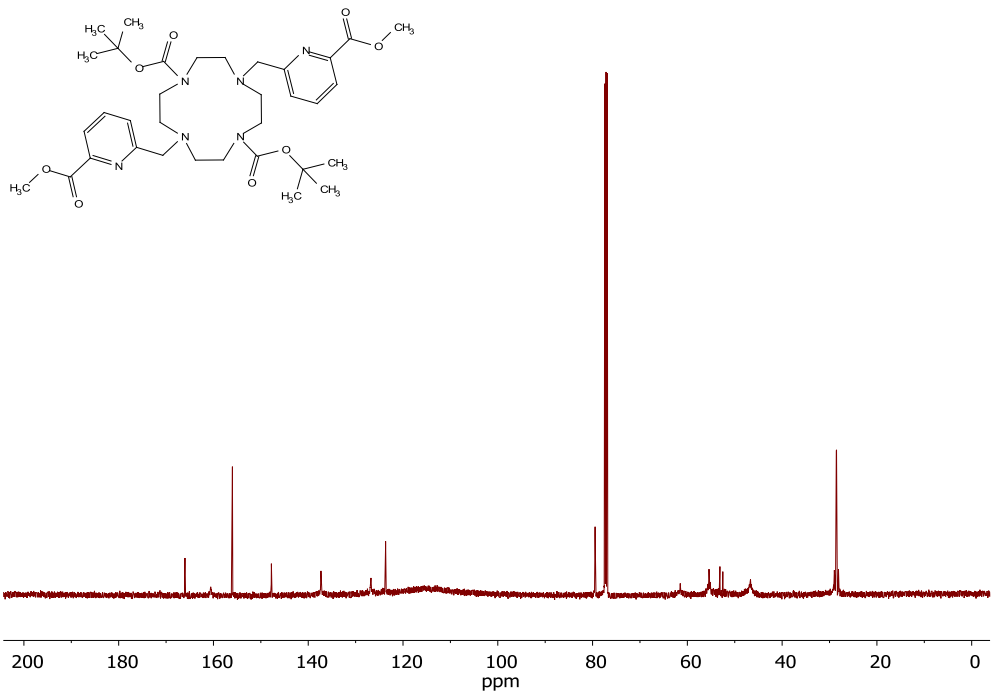


Di – *tert* - butil 4,10-bis ((6-(metoxicarbonil)piridina – 2 - il)metil) - 1,4,7,10-tetraazaciclododecano - 1,7 - dicarboxilato (**16**)

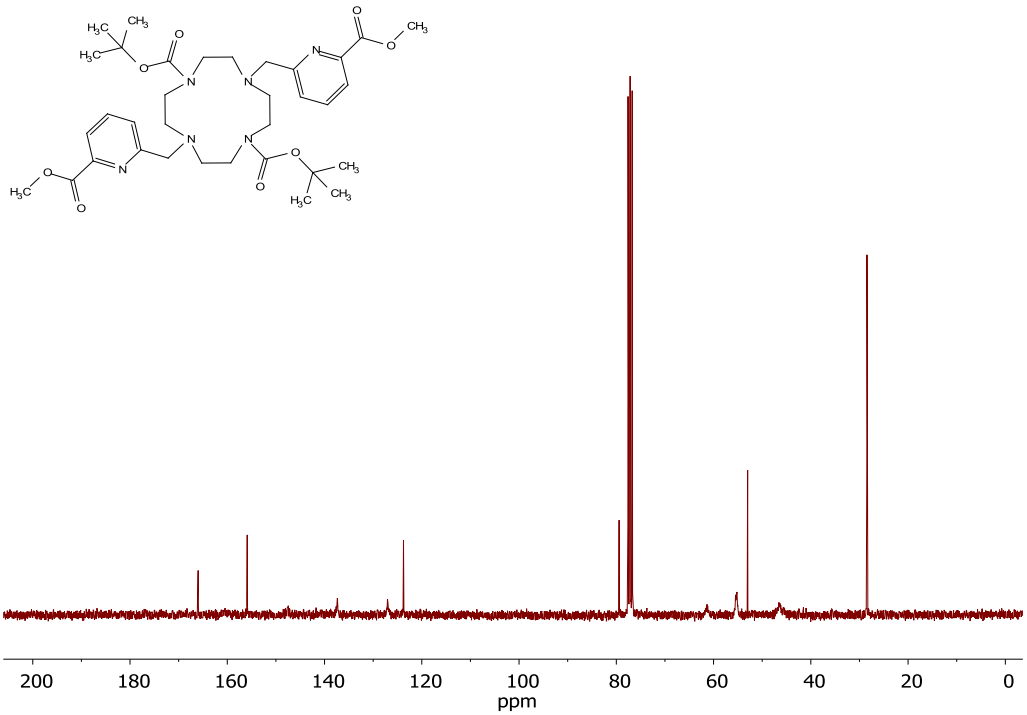
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



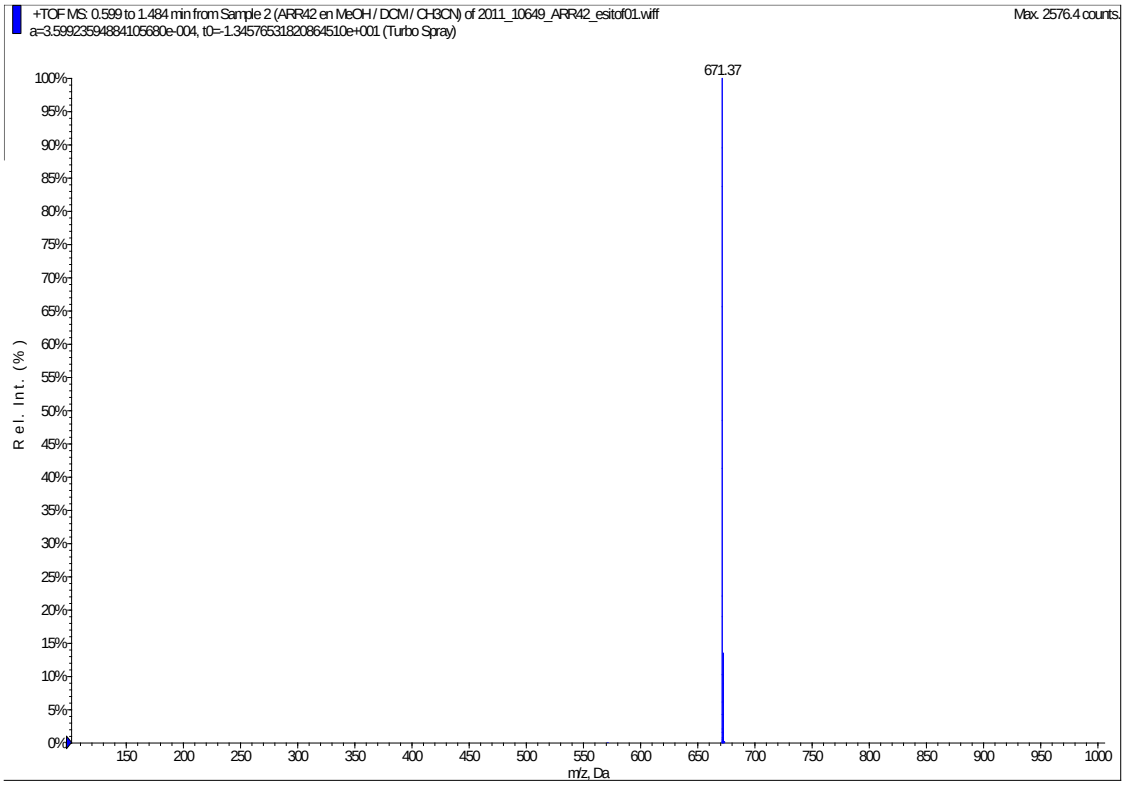
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm) (328,5 K), sonda bbi



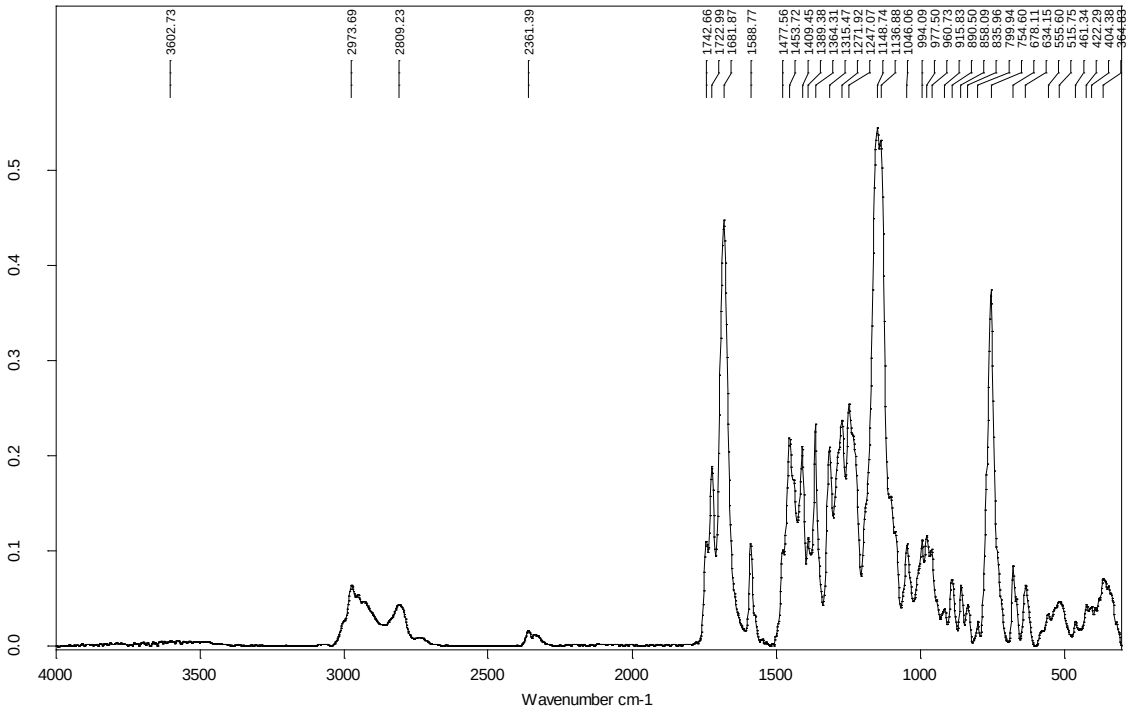
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



Espectro de masas ESI$^+$

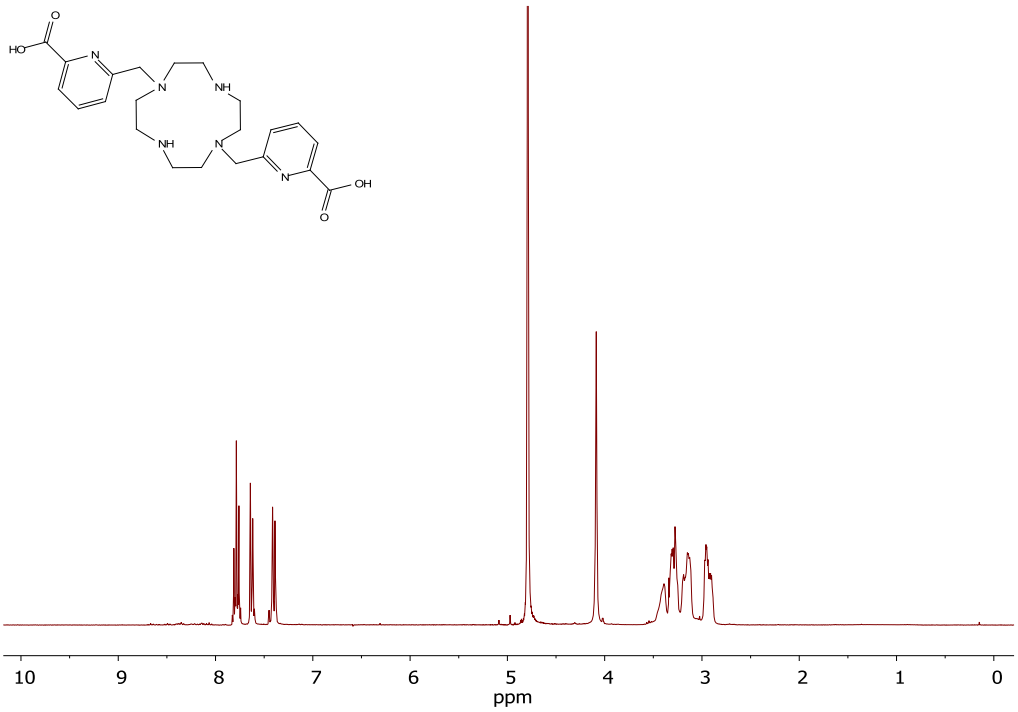


Espectro IR

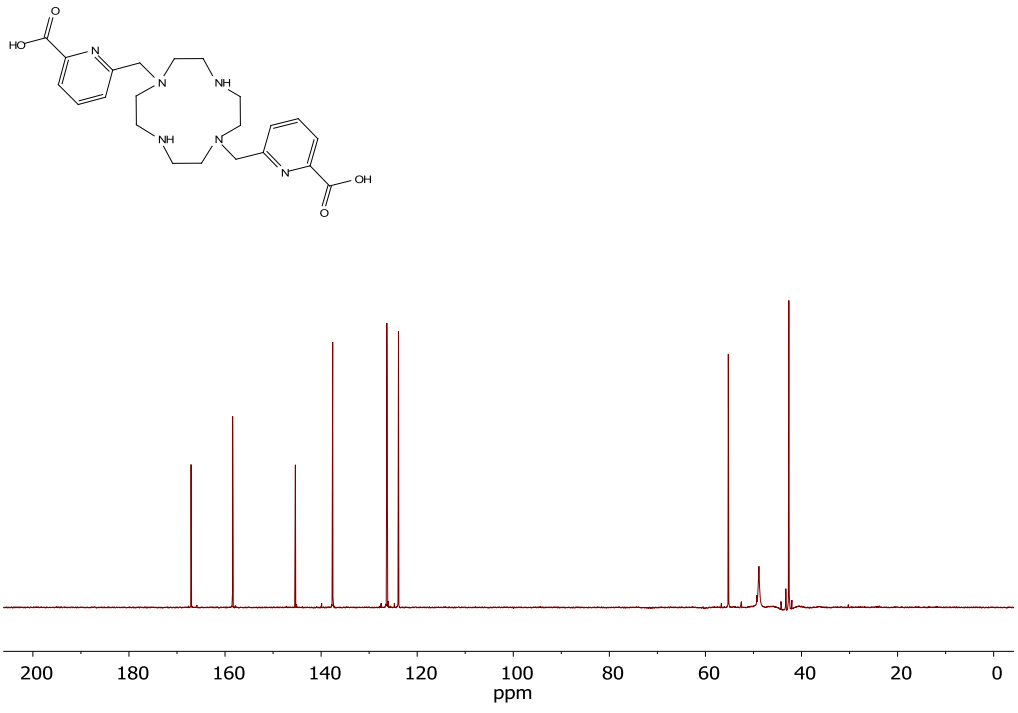

3602.73
2973.69
2809.23
2361.39
1742.66
1722.99
1681.87
1588.77
1477.56
1453.72
1409.45
1389.38
1364.31
1315.47
1271.92
1247.07
1148.74
1136.88
1046.06
994.09
977.50
960.73
915.83
890.50
858.09
835.96
799.84
754.60
678.11
634.15
555.60
515.75
461.34
422.29
404.38
364.68
0.0
0.1
0.2
0.3
0.4
0.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Ácido 6,6´ - ((1,4,7,10 – tetraazaciclododecano - 1,7 - diil) bis -(metilen))dipicolínico (H_2**dodpa·5HCl·4H_2O**)

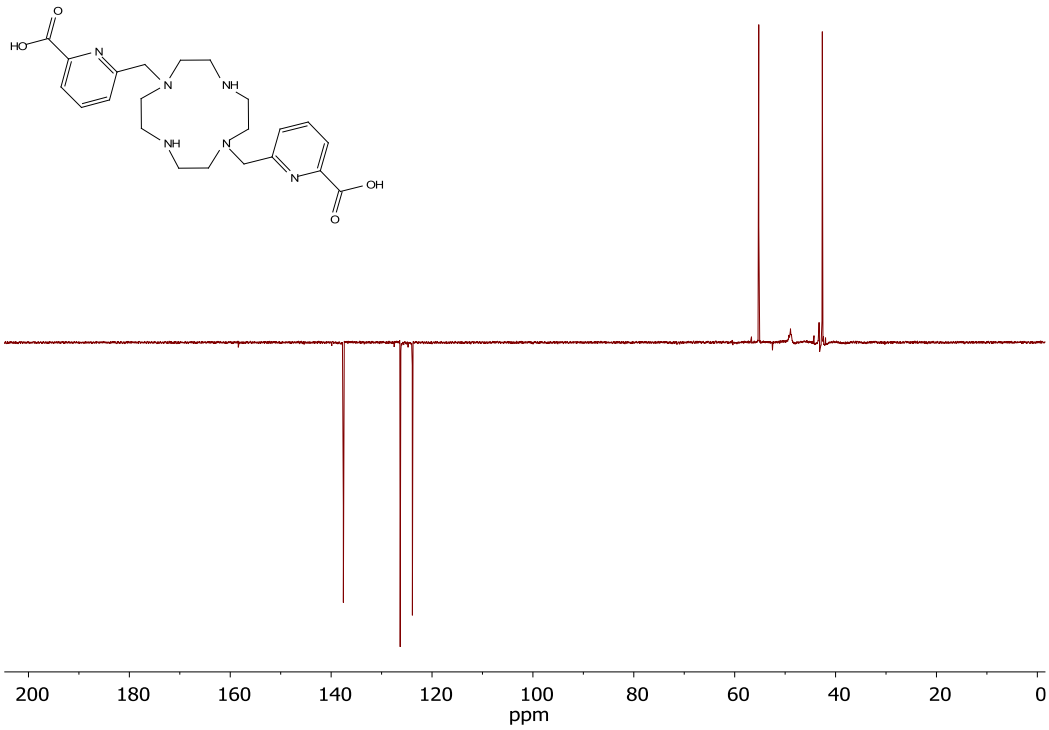
^{1}H-RMN (D_2O, 500 MHz, pD = 0,7) (δ/ppm)



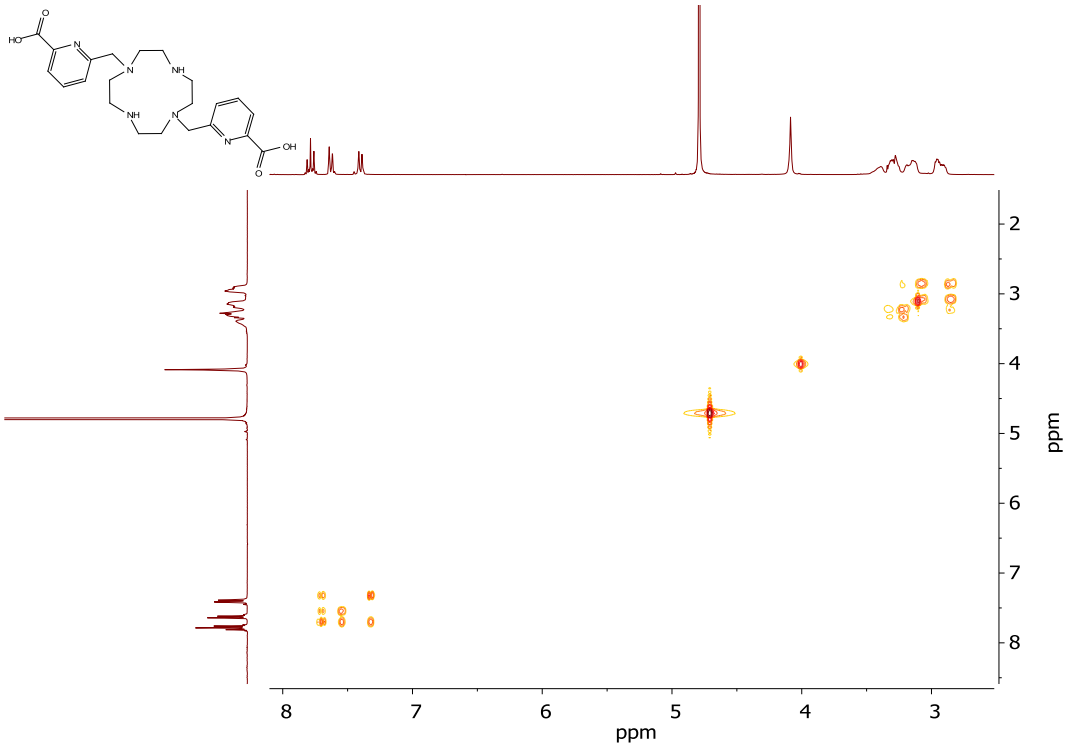
^{13}C-RMN (D_2O, 125,8 MHz, pD = 0,7) (δ/ppm)



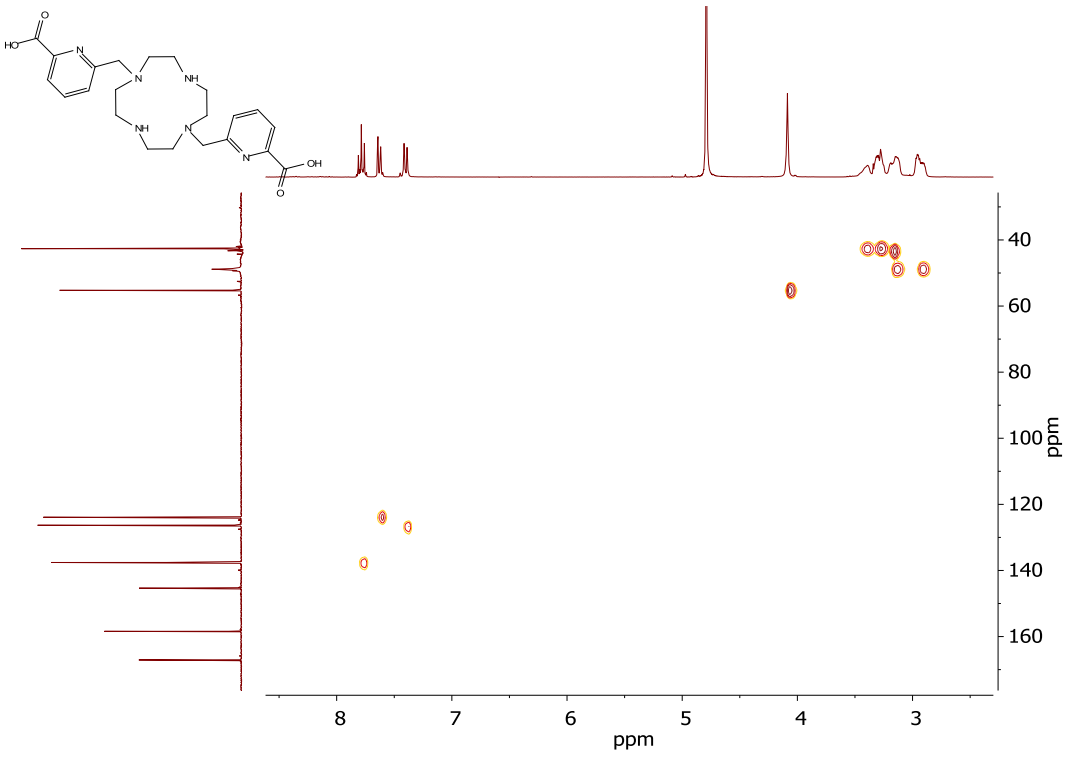
DEPT-RMN (D_2O, pD = 0,7) (δ/ppm)



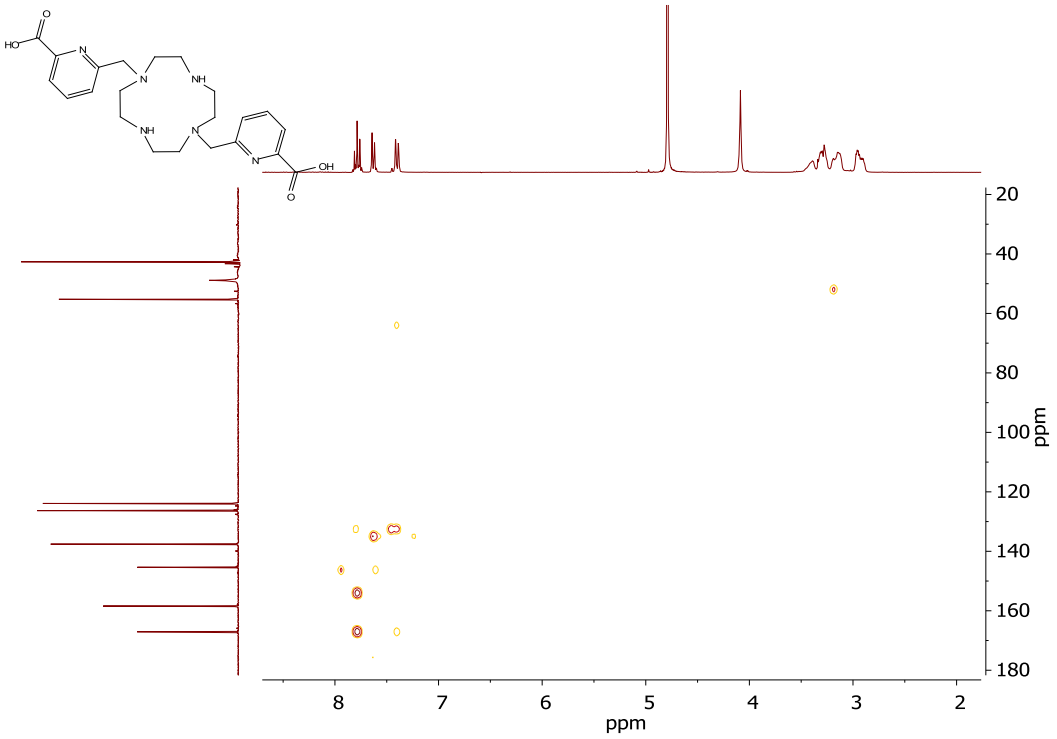
COSY-RMN (D_2O, pD = 0,7) (δ/ppm)



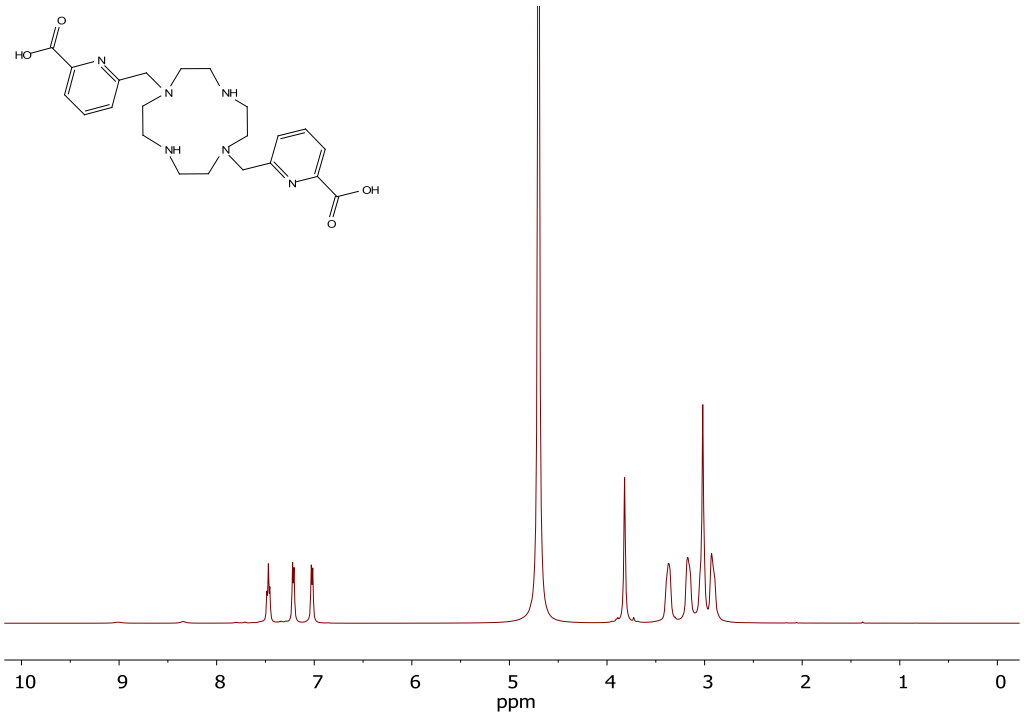
HSQC-RMN (D_2O, pD = 0,7) (δ/ppm)



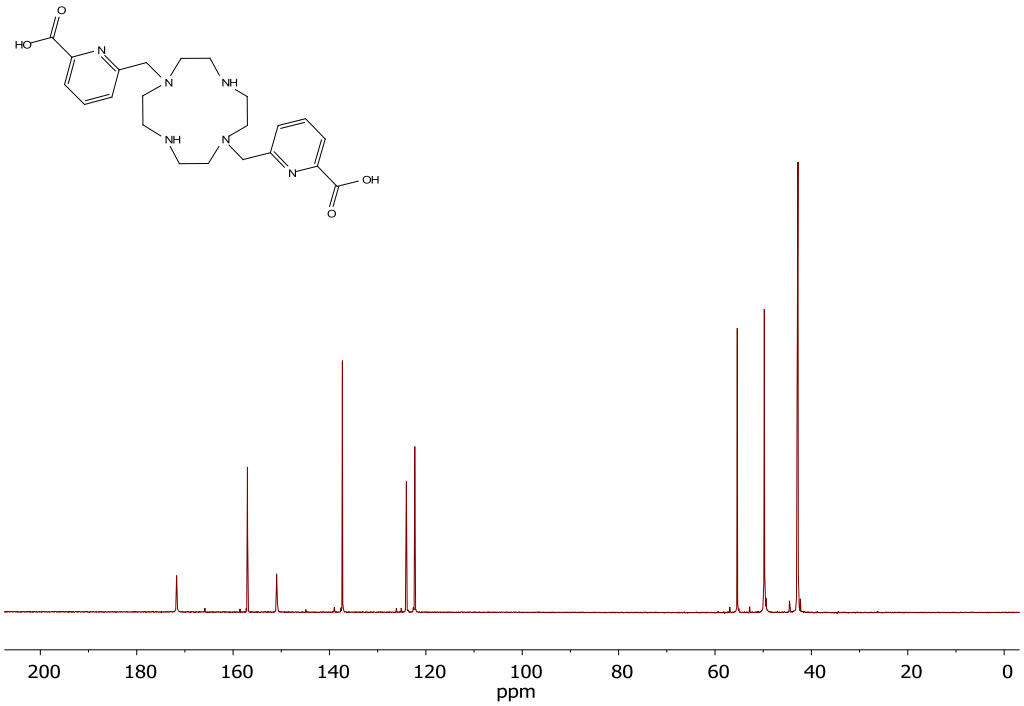
HMBC-RMN (D_2O, pD = 0,7) (δ/ppm)



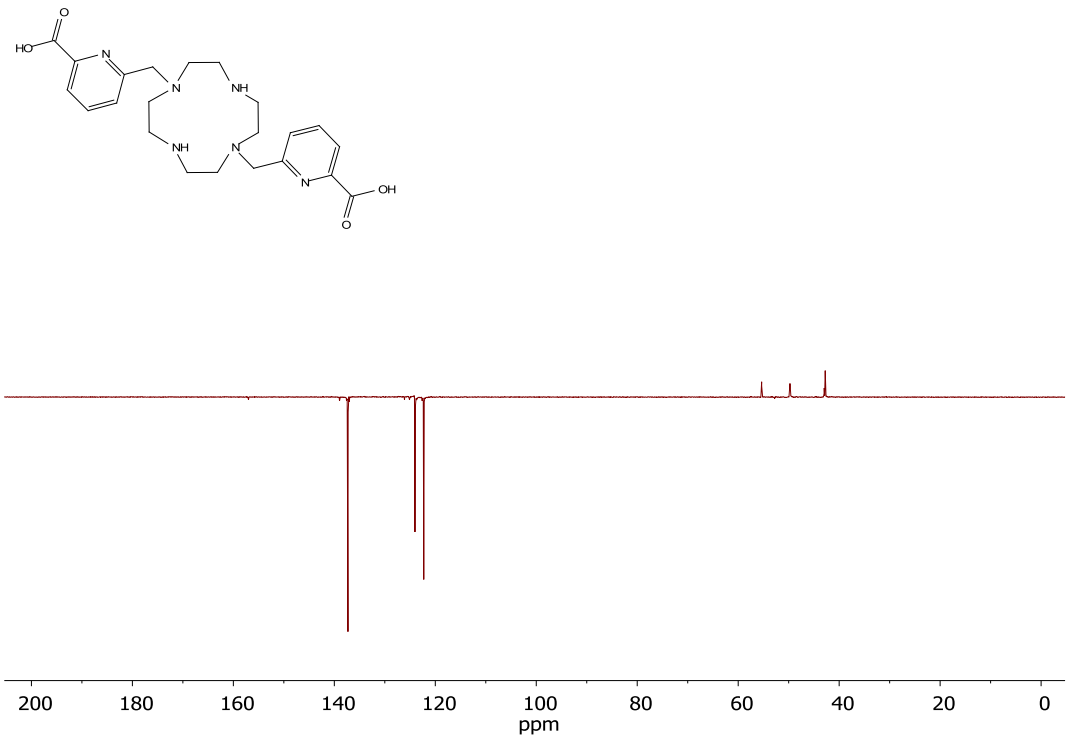
^{1}H-RMN (D_2O, 500 MHz, pD = 7,1) (δ/ppm)



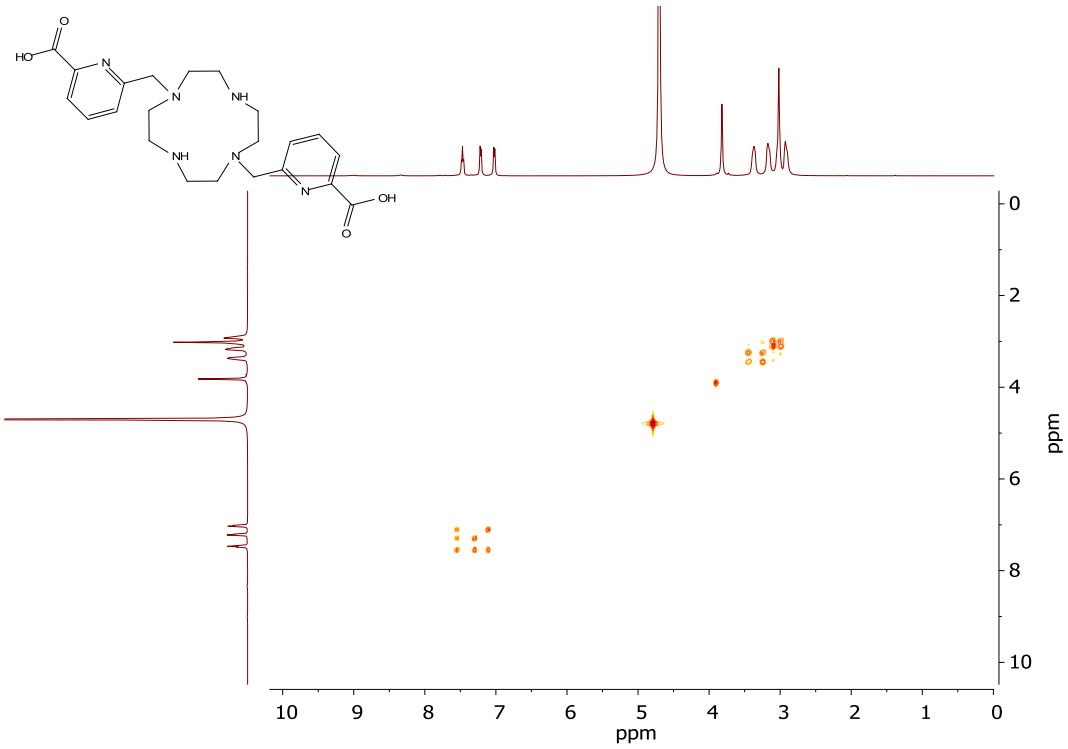
^{13}C-RMN (D_2O, 125,8 MHz, pD = 7,1) (δ/ppm)



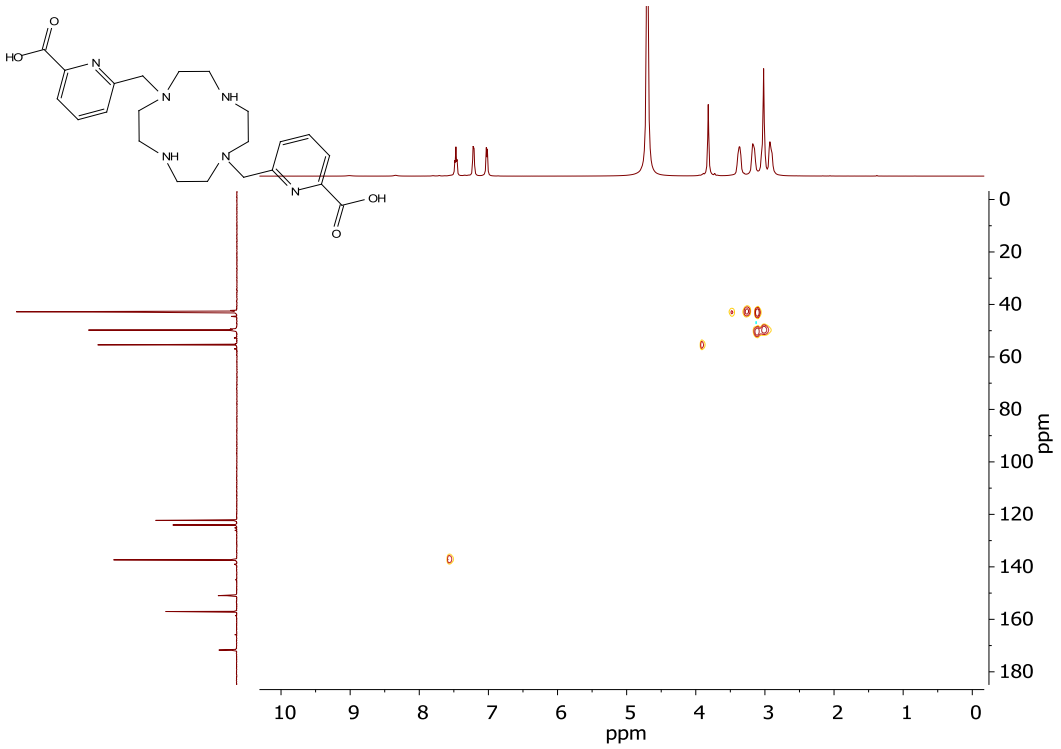
DEPT-RMN (D_2O, pD = 7,1) (δ/ppm)



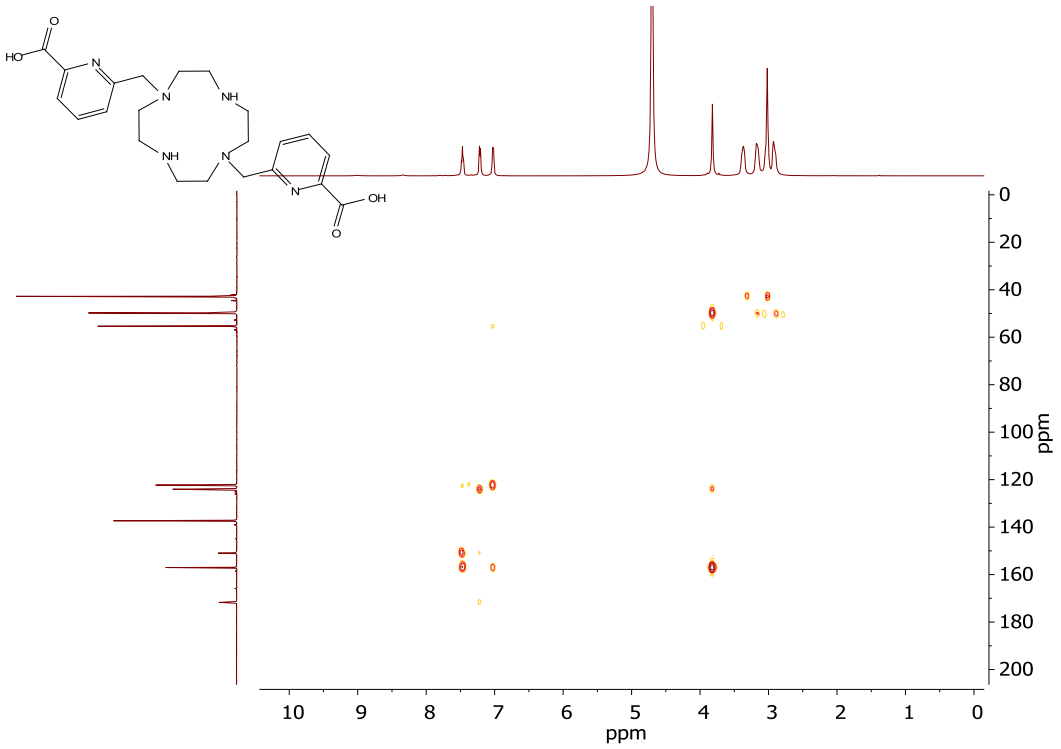
COSY-RMN (D_2O, pD = 7,1) (δ/ppm)



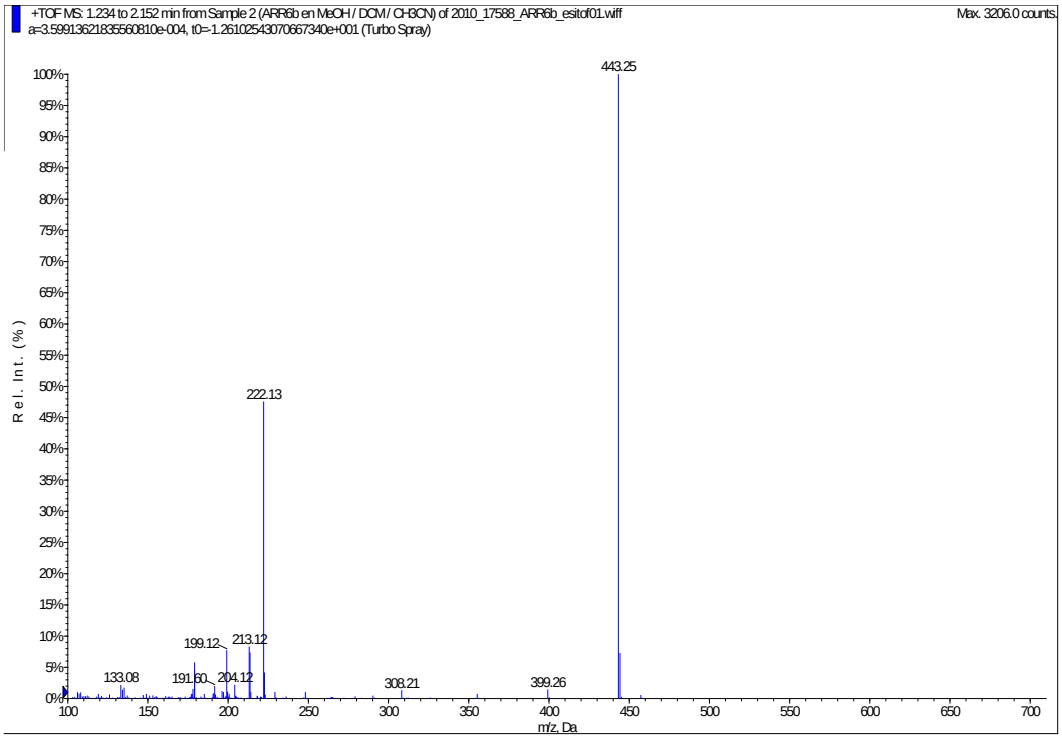
HSQC-RMN (D_2O, pD = 7,1) (δ/ppm)



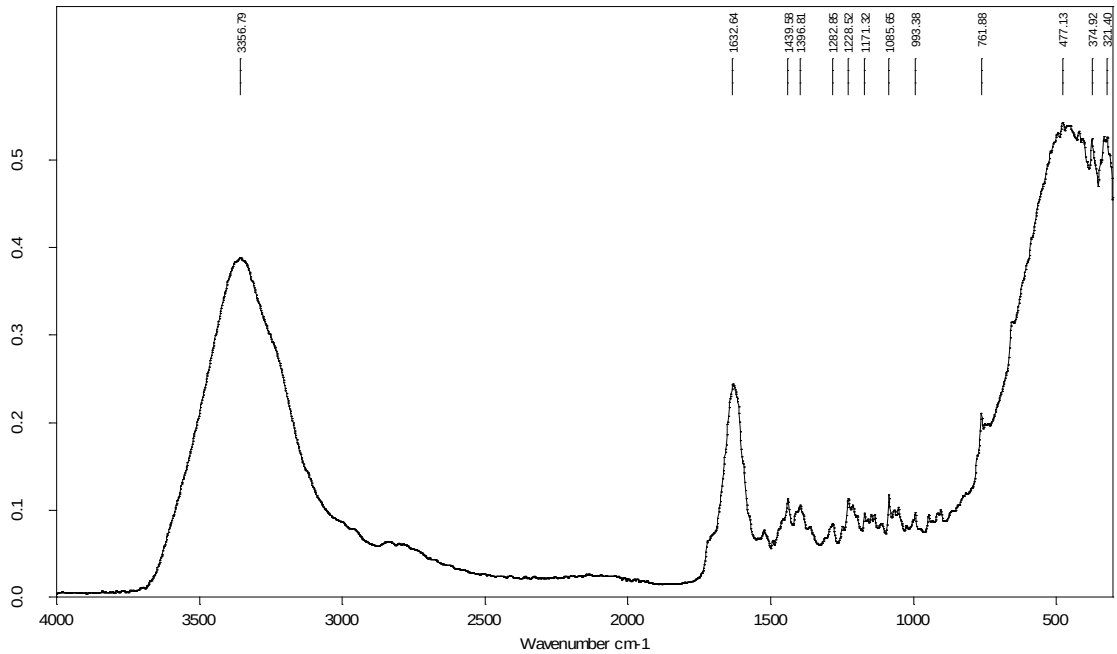
HMBC-RMN (D_2O, pD = 7,1) (δ/ppm)



Espectro de masas ESI+

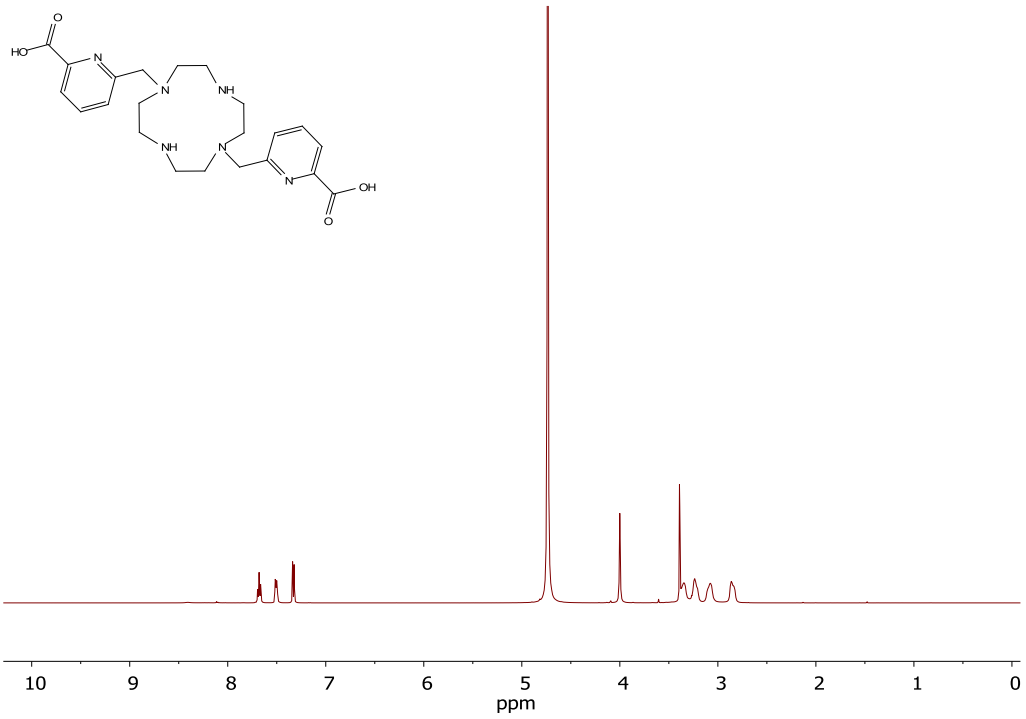


Espectro IR

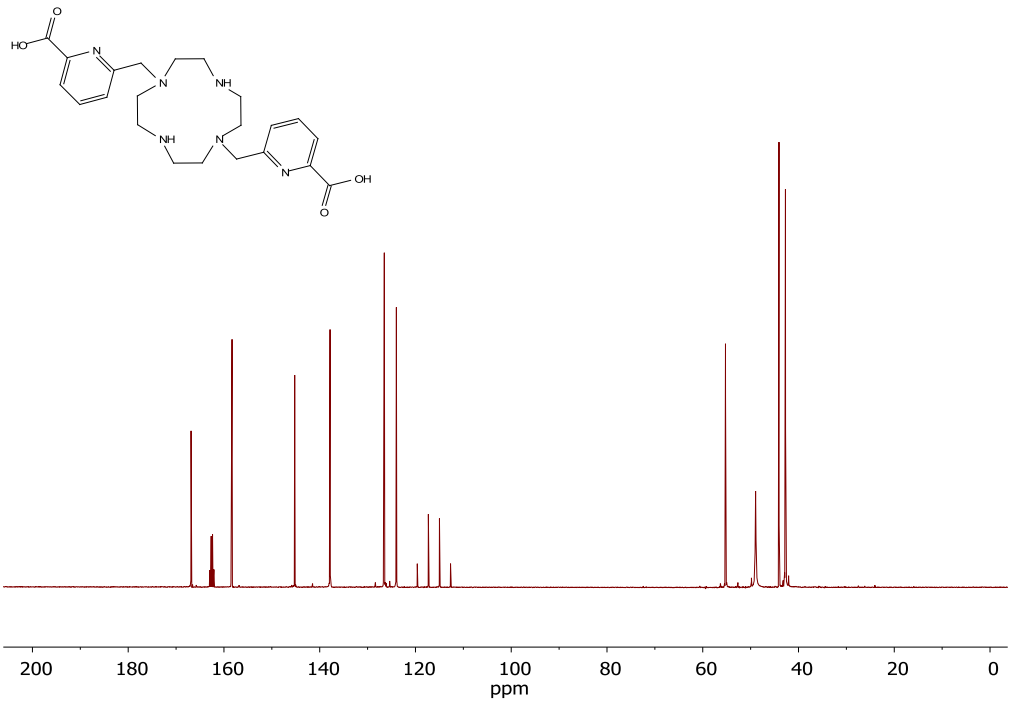


Ácido 6,6´ - ((1,4,7,10 – tetraazaciclododecano - 1,7 - diil) bis -(metilen))dipicolínico (**H_2dodpa·5TFA**)

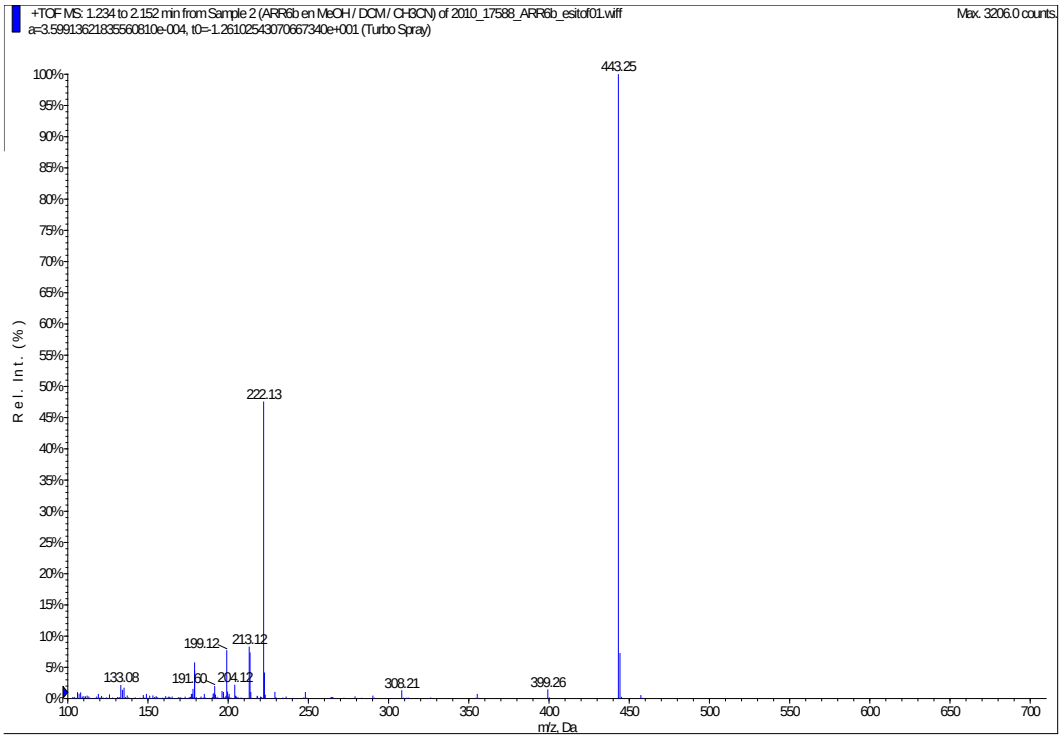
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



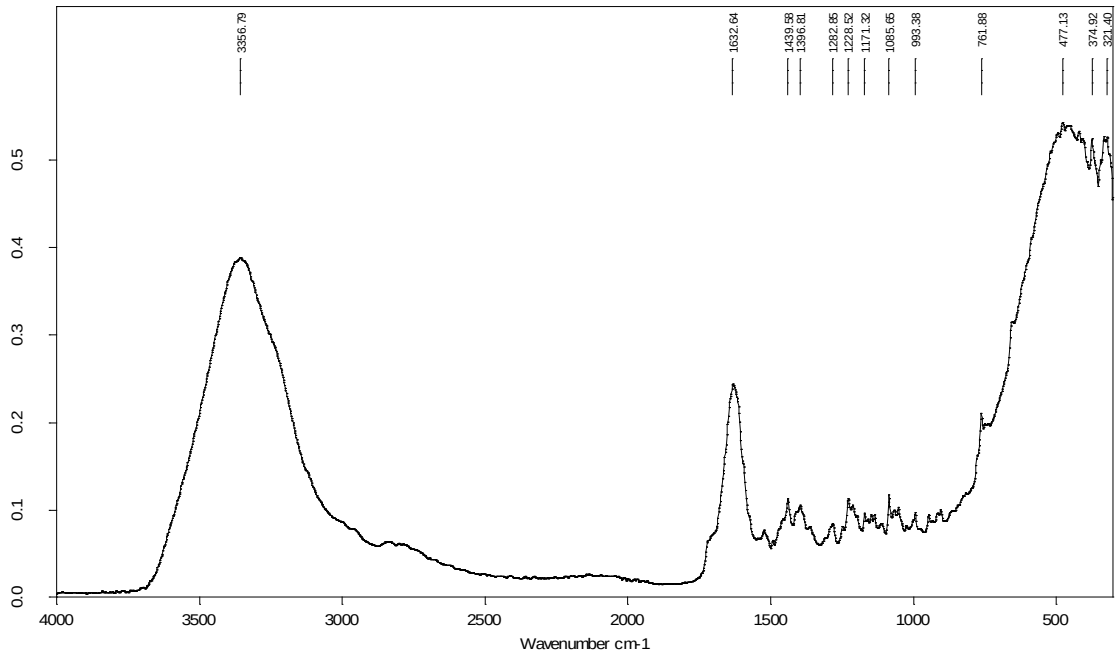
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



Espectro de masas ESI+

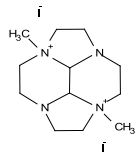


Espectro IR

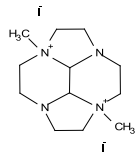


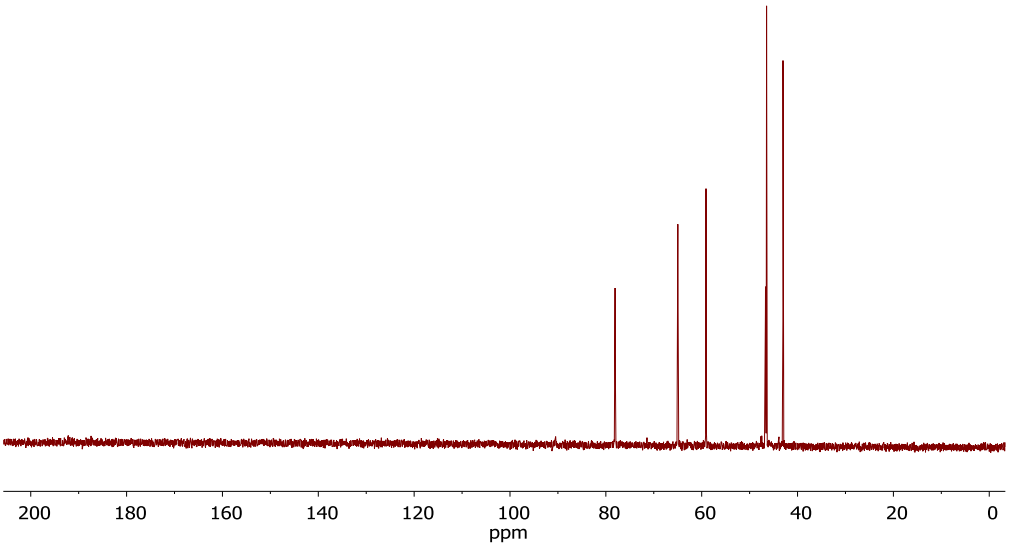
2a,6a - Diyoduro de 2a,6a – dimetildodecahidro - 2a,4a,6a,8a – tetraazaciclopenta [*fg*] acenaftileno (**17**)

^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)

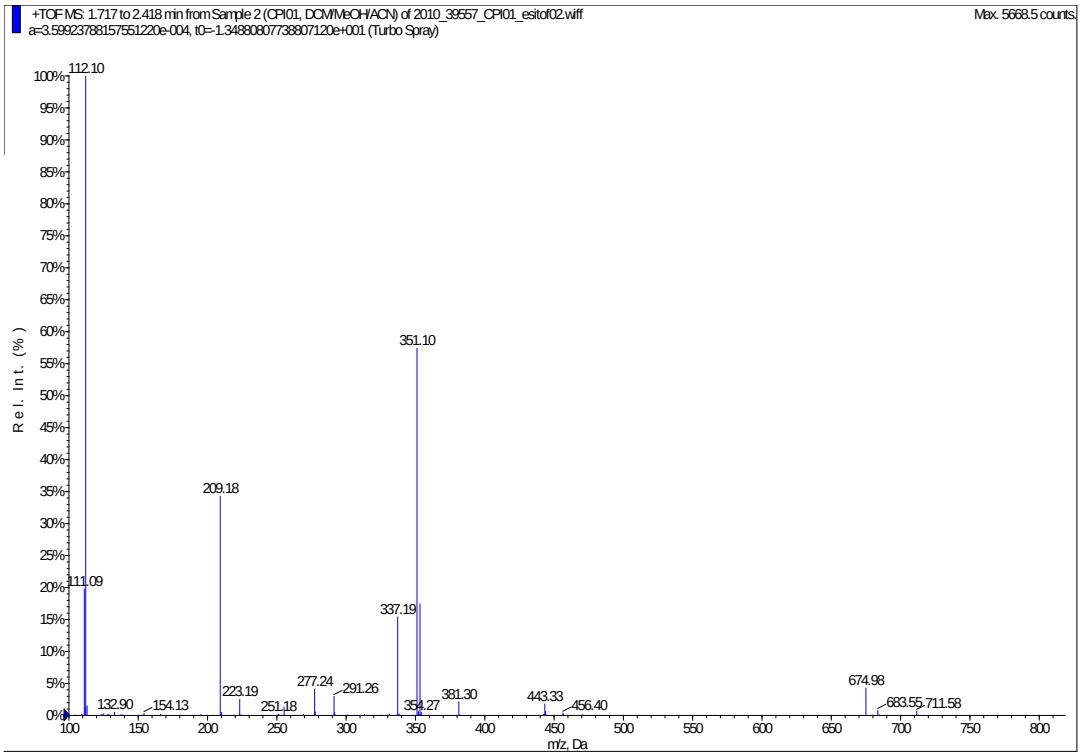


^{13}C-RMN (D2O, 75,5 MHz) (δ/ppm)

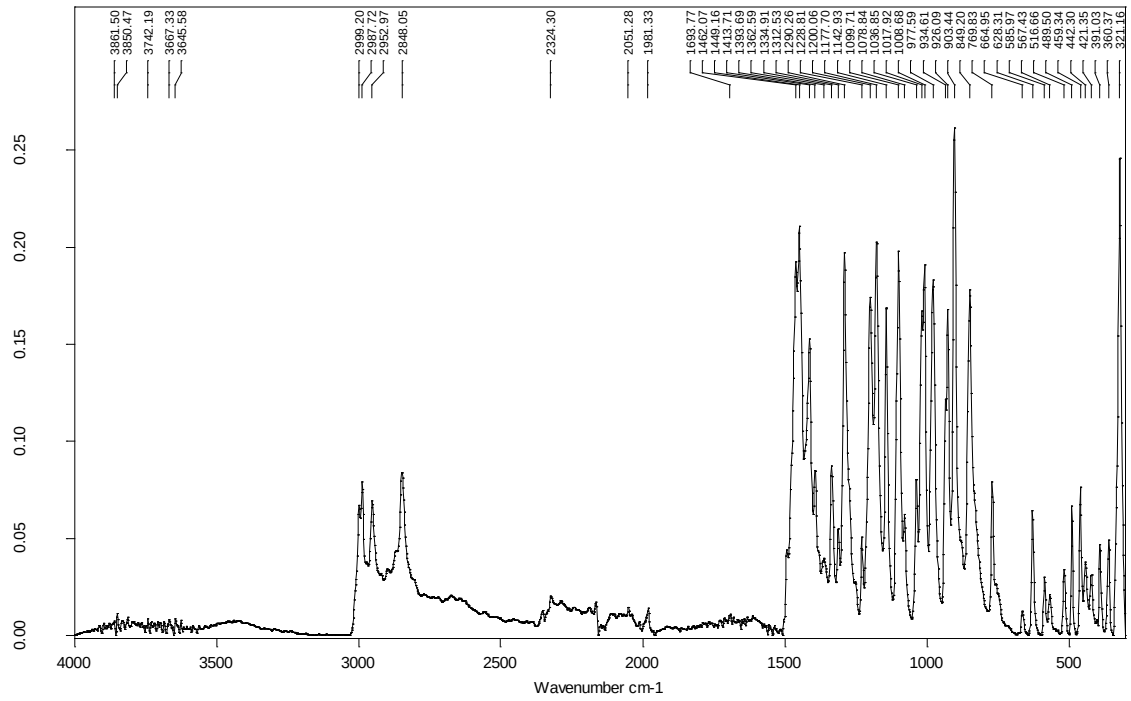




Espectro de masas ESI+

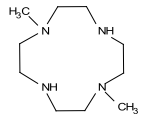


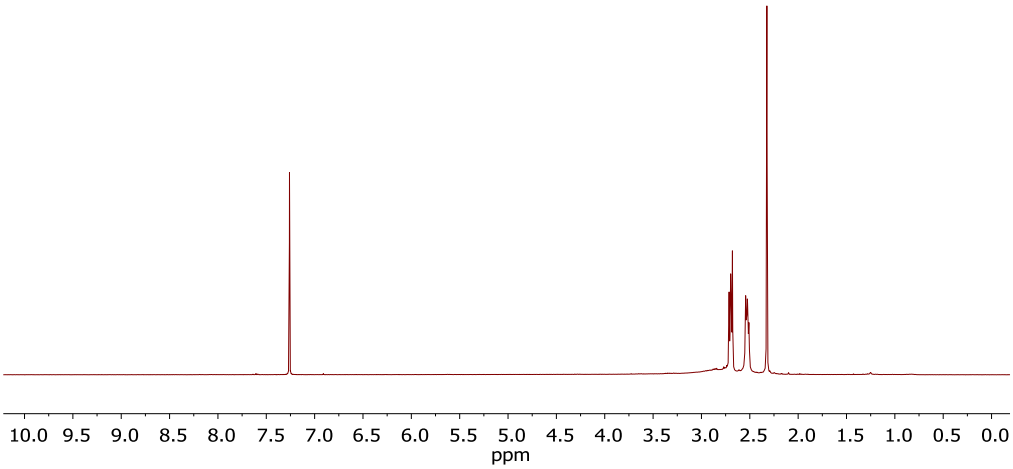
Espectro IR



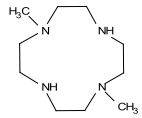
1,7-Dimetil-1,4,7,10-tetraazaciclododecano (**18**)

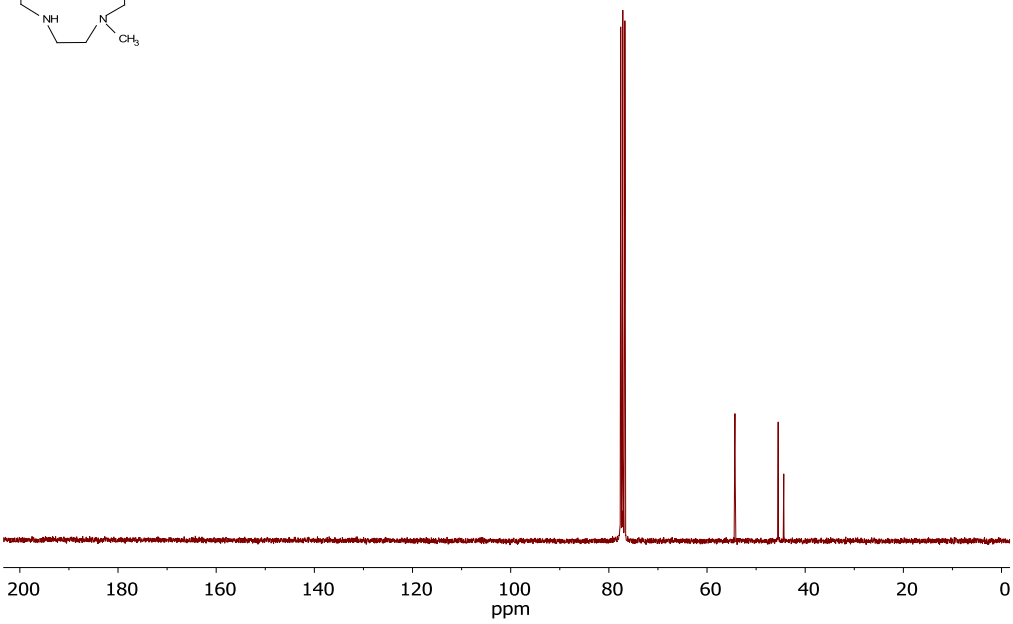
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



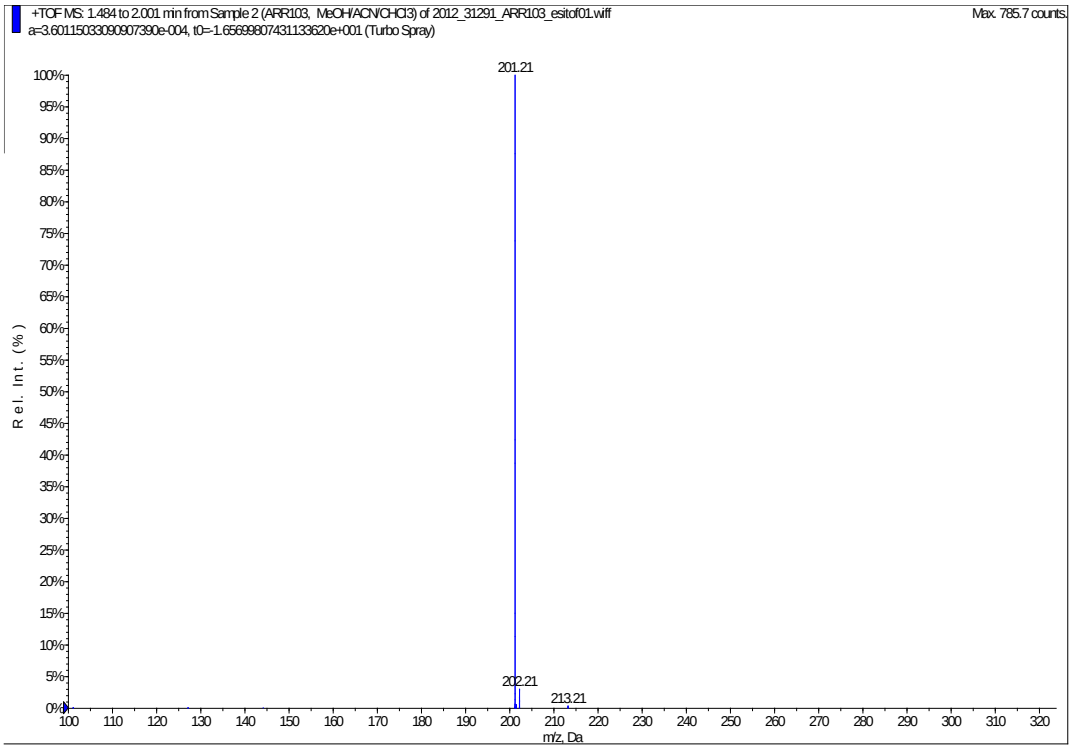


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

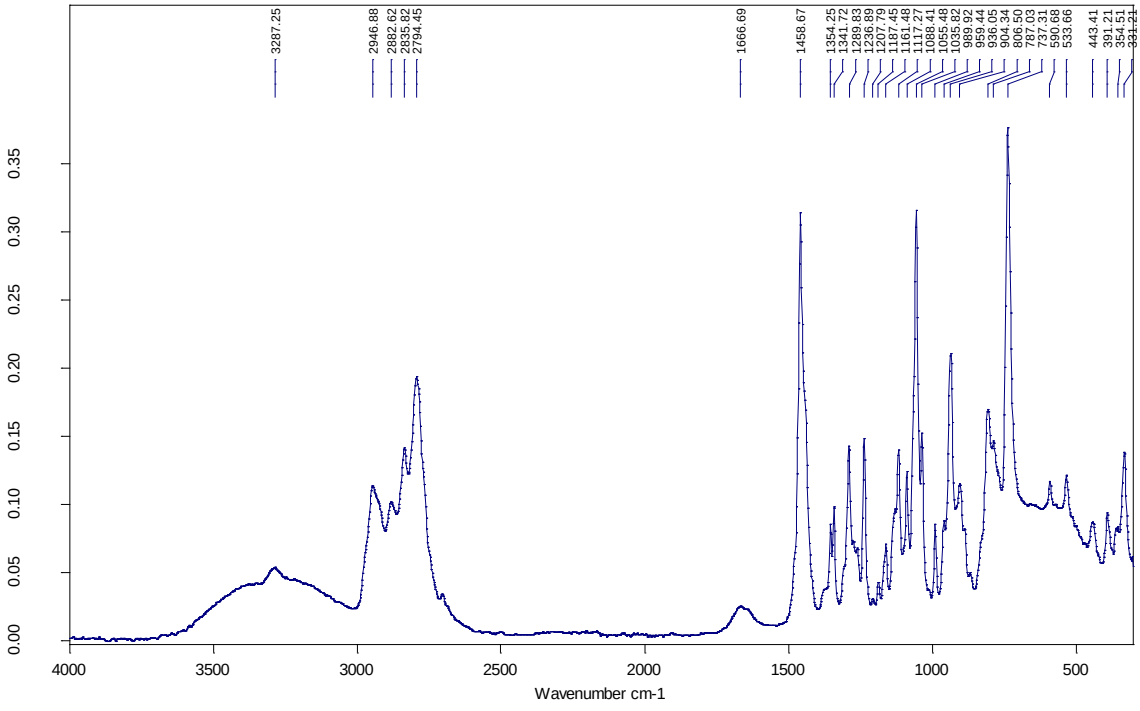




Espectro de masas ESI+

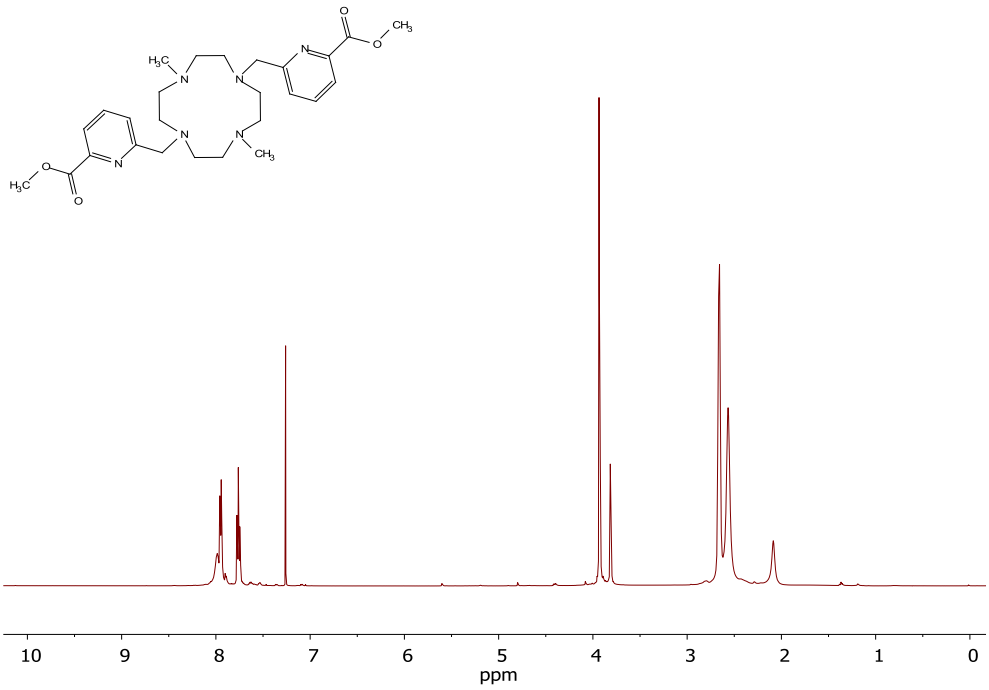


Espectro IR

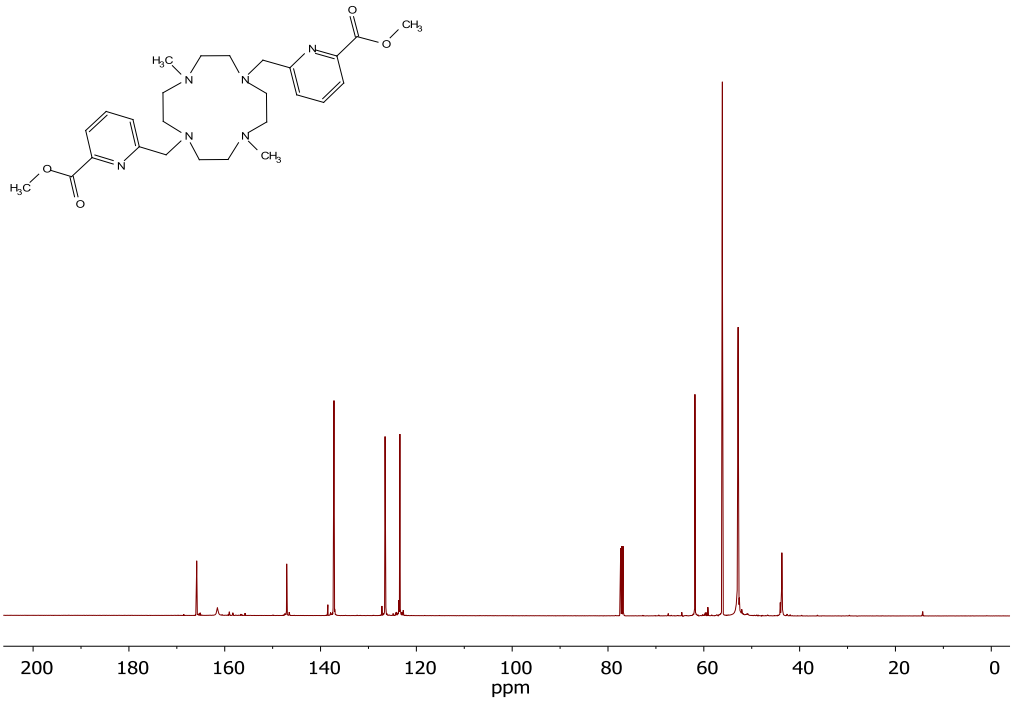


Dimetil 6,6´ - ((4,10 – dimetil - 1,4,7,10 – tetraazaciclododecano - 1,7 - diil)bis(metilen))dipicolinato (**19**)

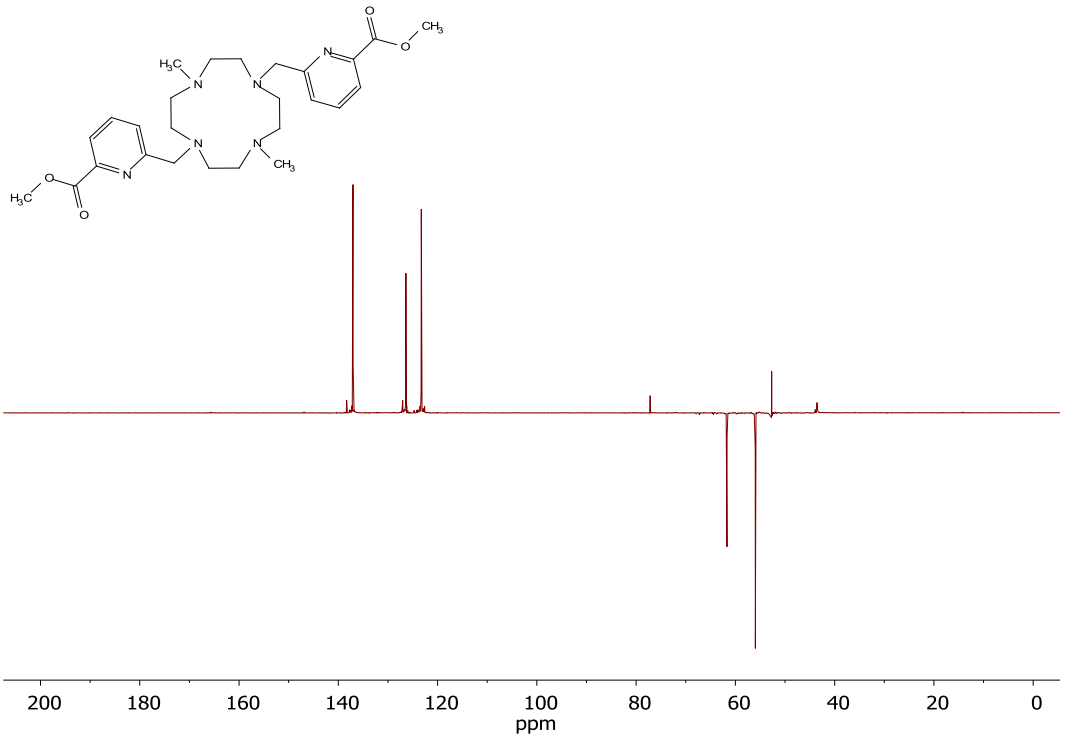
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



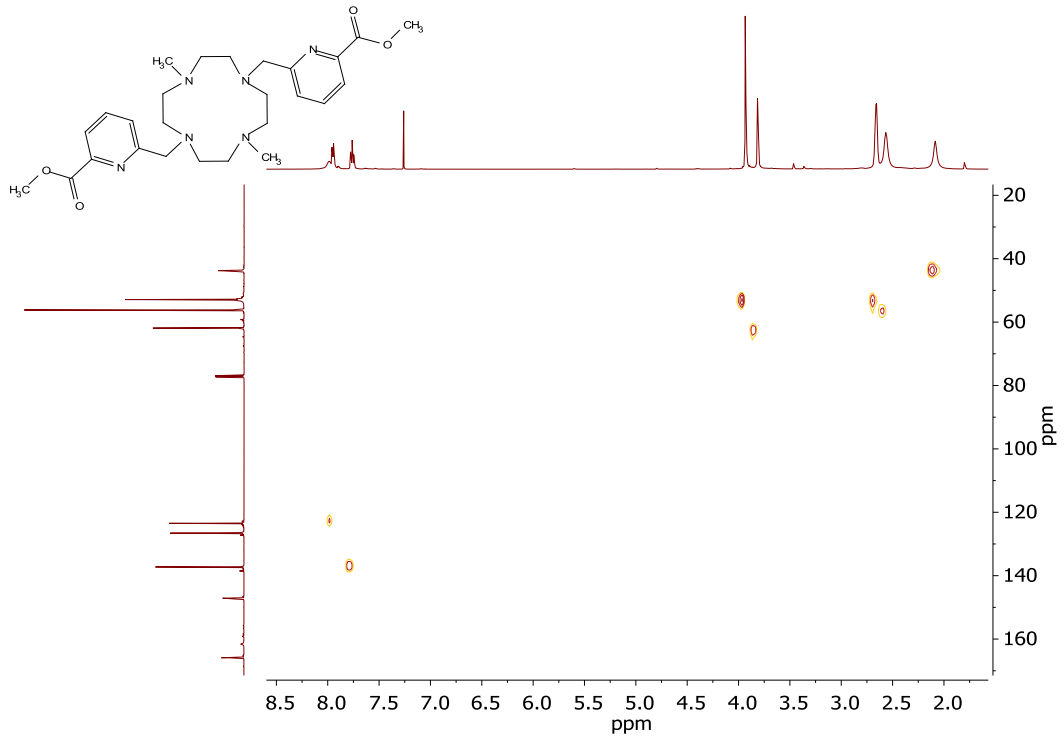
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



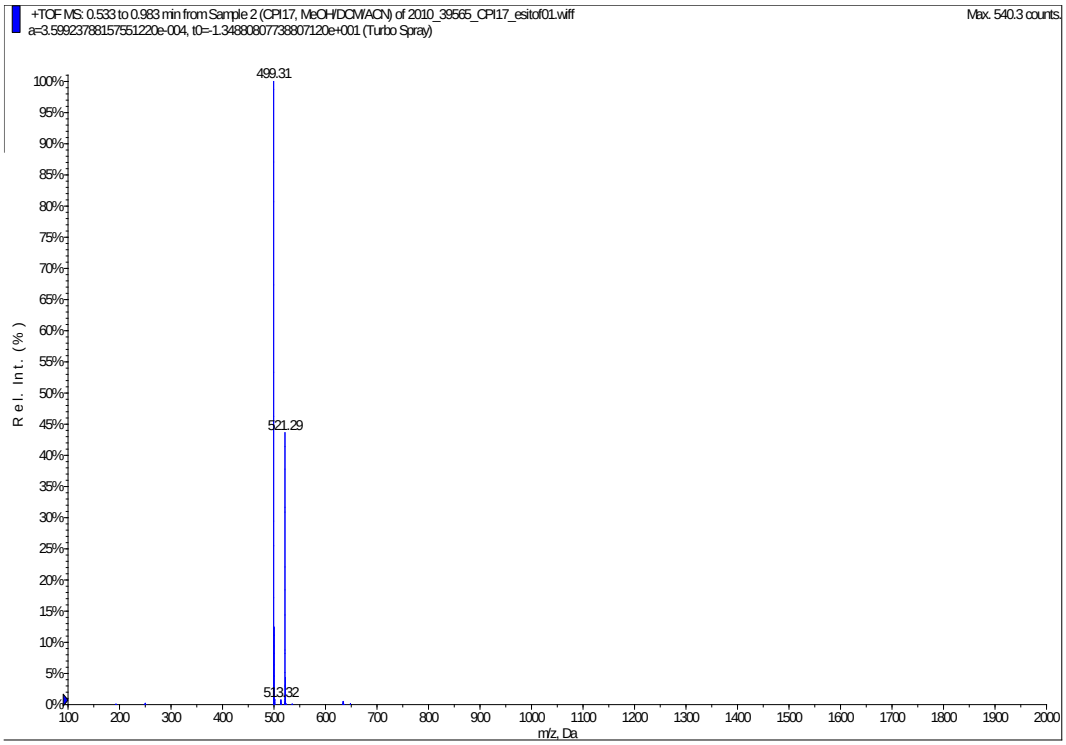
DEPT-RMN ($CDCl_3$) (δ/ppm)



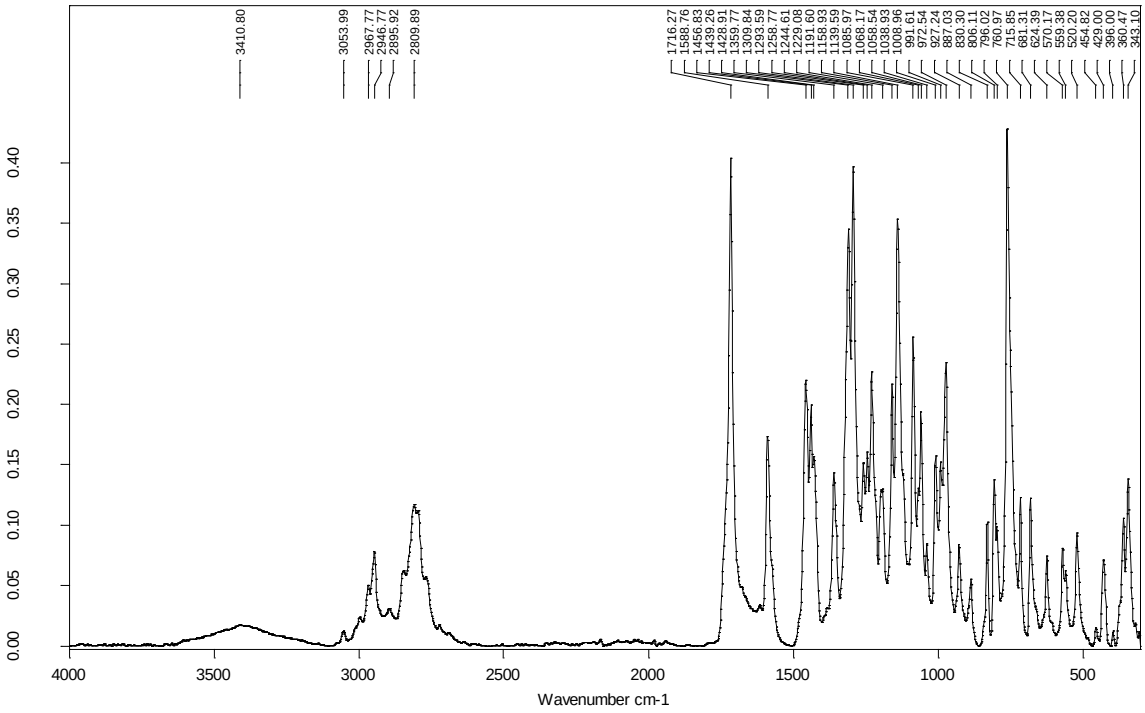
HSQC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

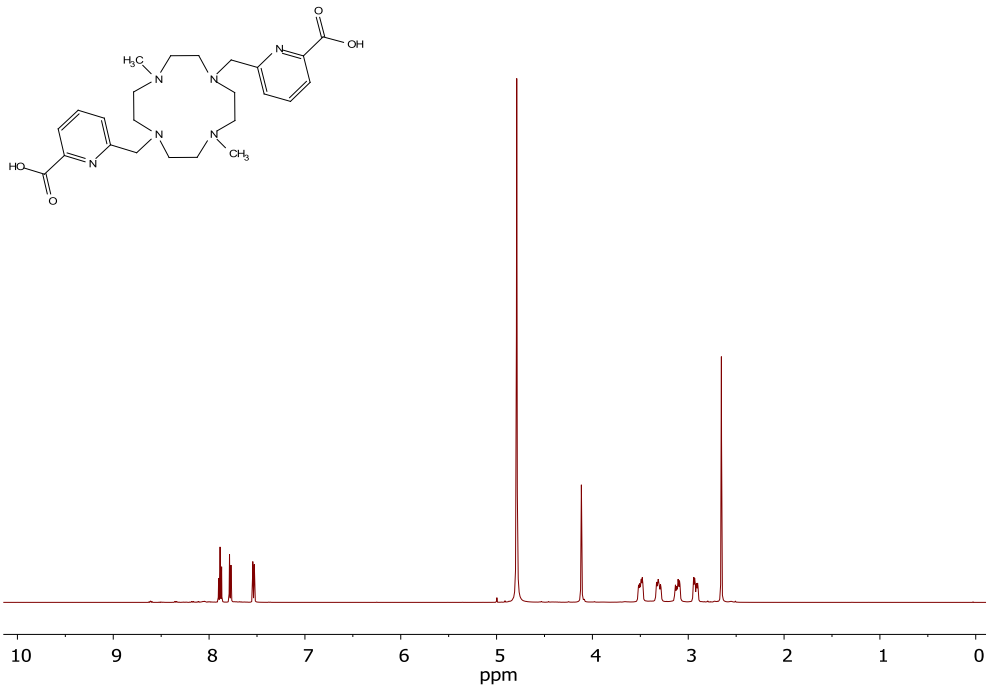


Espectro IR

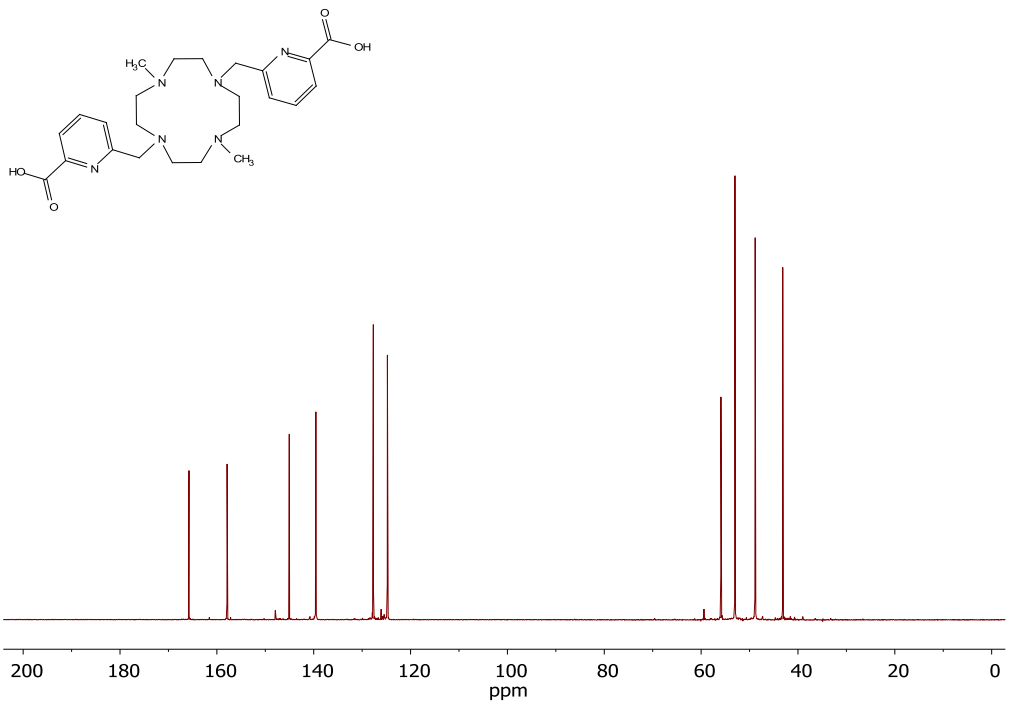


Ácido dimetil 6,6´ - ((4,10 – dimetil - 1,4,7,10 – tetraazaciclododecano - 1,7 - diil)bis(metilen))dipicolínico ($H_2Me_2DODPA·7HCl·H_2O$)

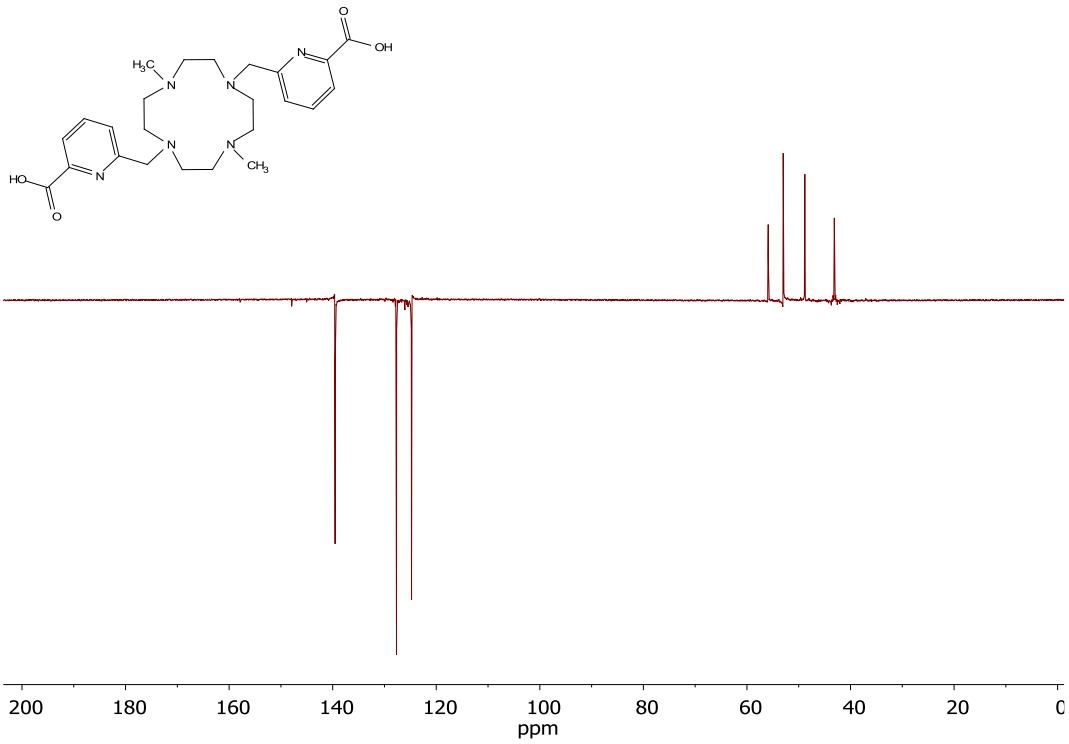
^{1}H-RMN (D_2O, 500 MHz, pD = 0,8) (δ/ppm)



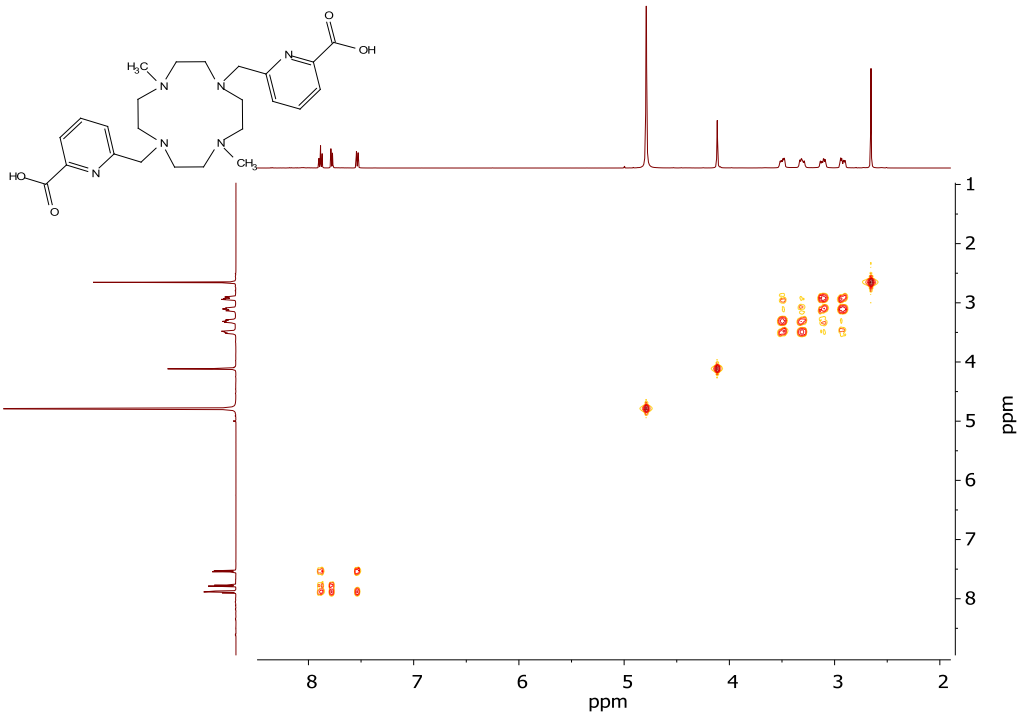
^{13}C-RMN (D_2O, 125,8 MHz, pD = 0,8) (δ/ppm)



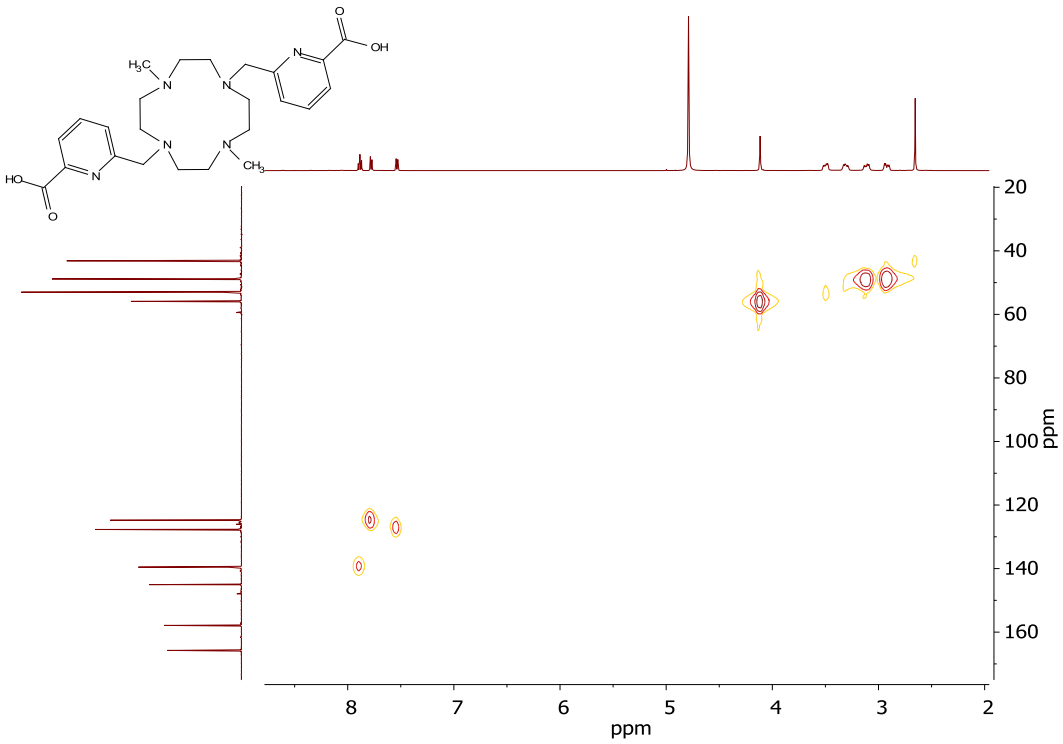
DEPT-RMN (D_2O, pD = 0,8) (δ/ppm)



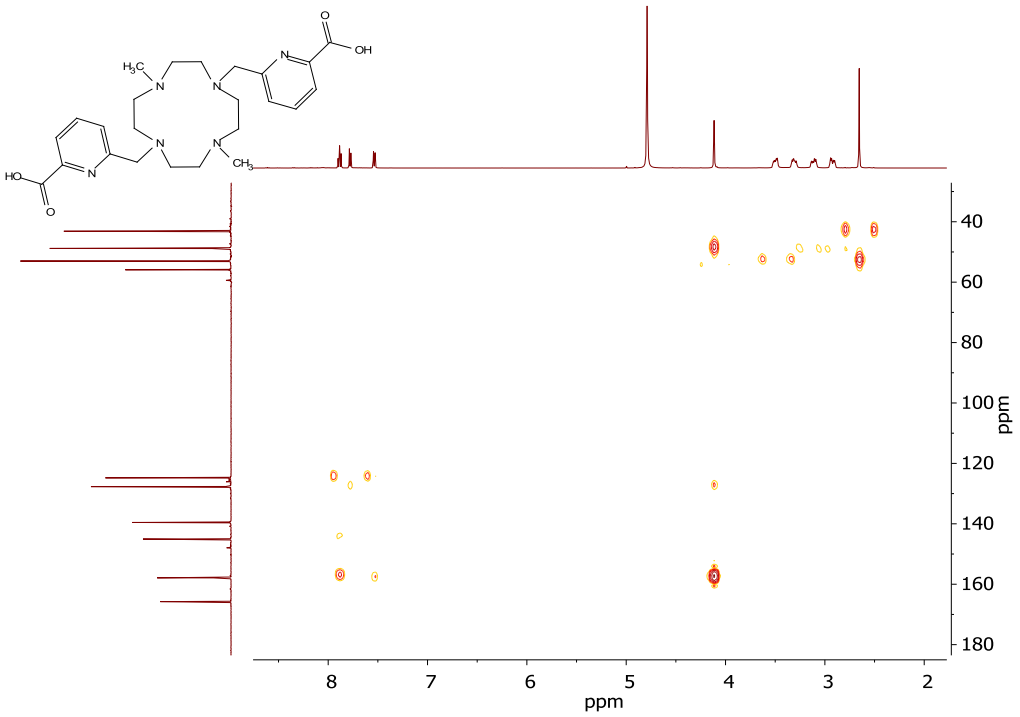
COSY-RMN (D_2O, pD = 0,8) (δ/ppm)



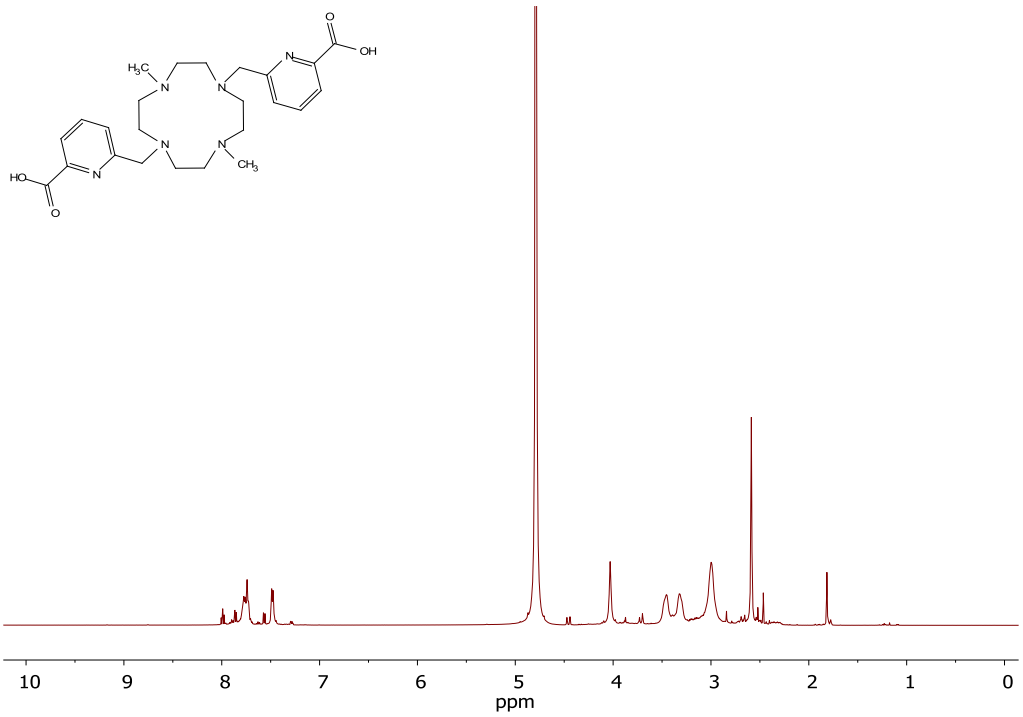
HSQC-RMN (D_2O, pD = 0,8) (δ/ppm)



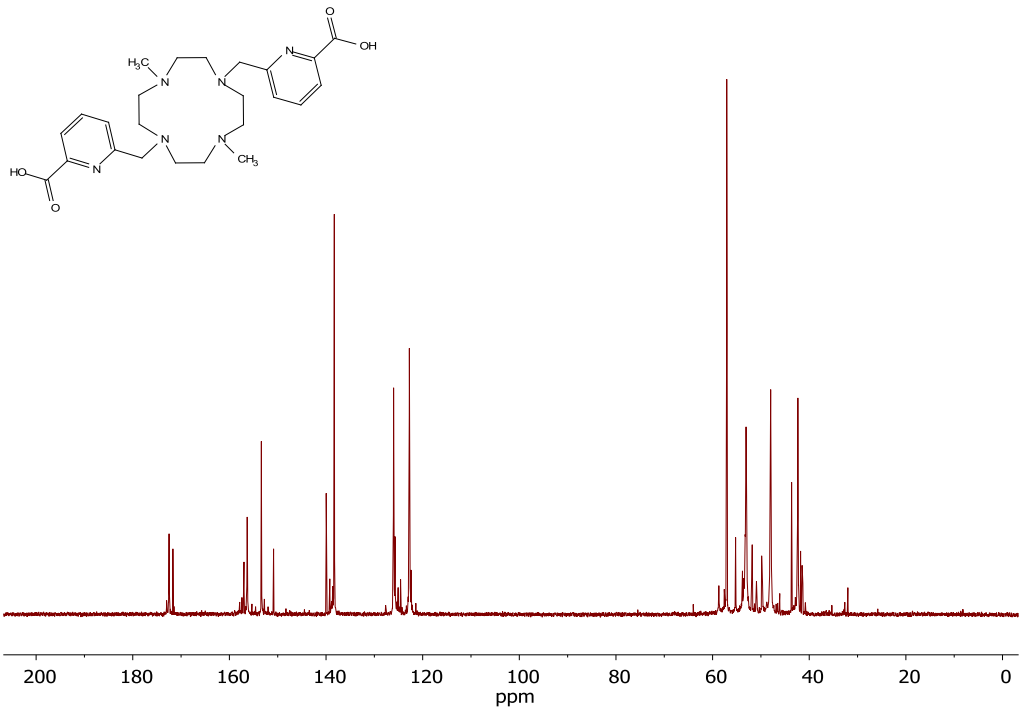
HMBC-RMN (D_2O, pD = 0,8) (δ/ppm)



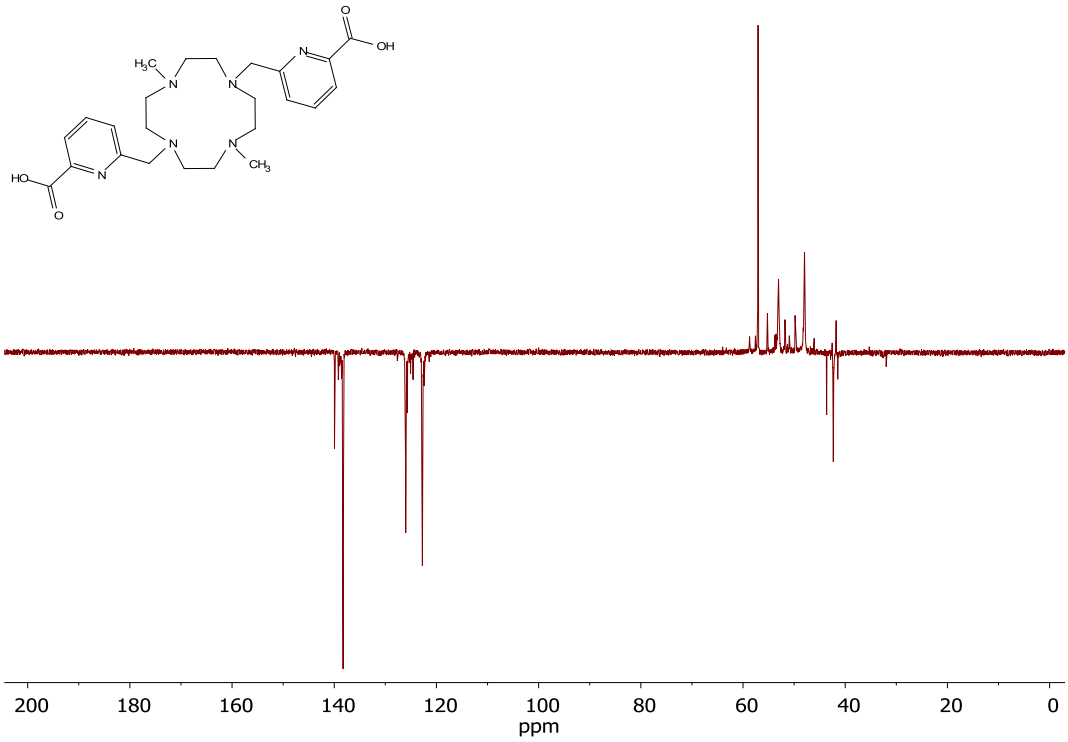
^{1}H-RMN (D_2O, 500 MHz, pD = 7,0) (δ/ppm)



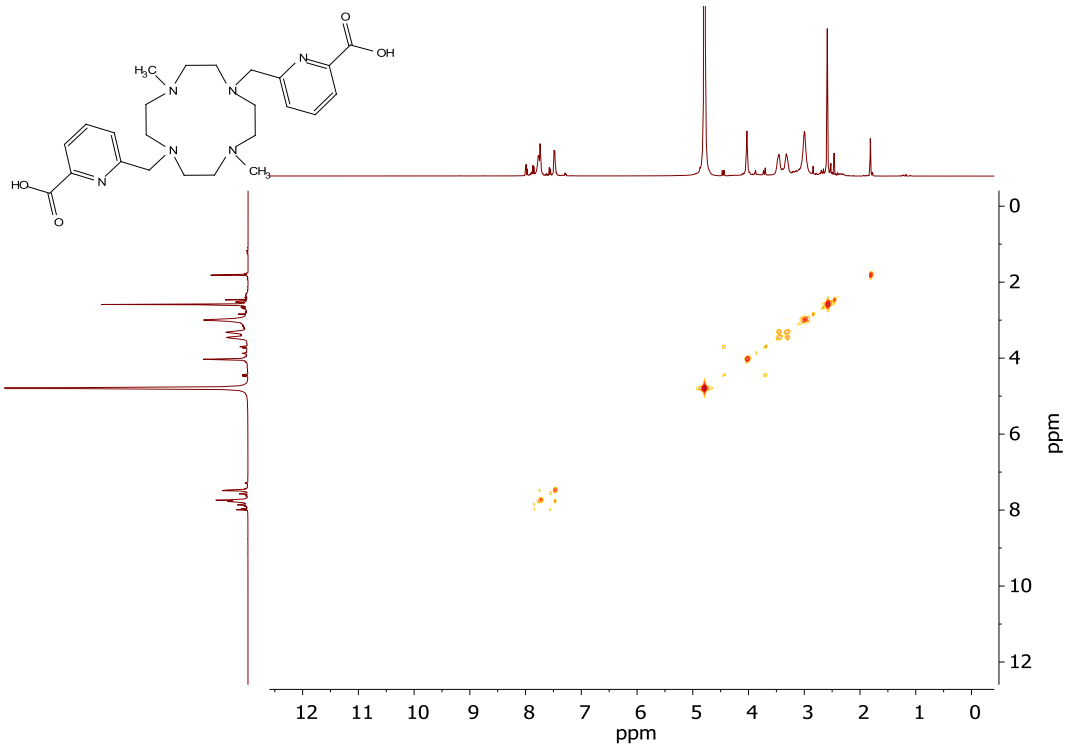
^{13}C-RMN (D_2O, 125,8 MHz, pD = 7,0) (δ/ppm)



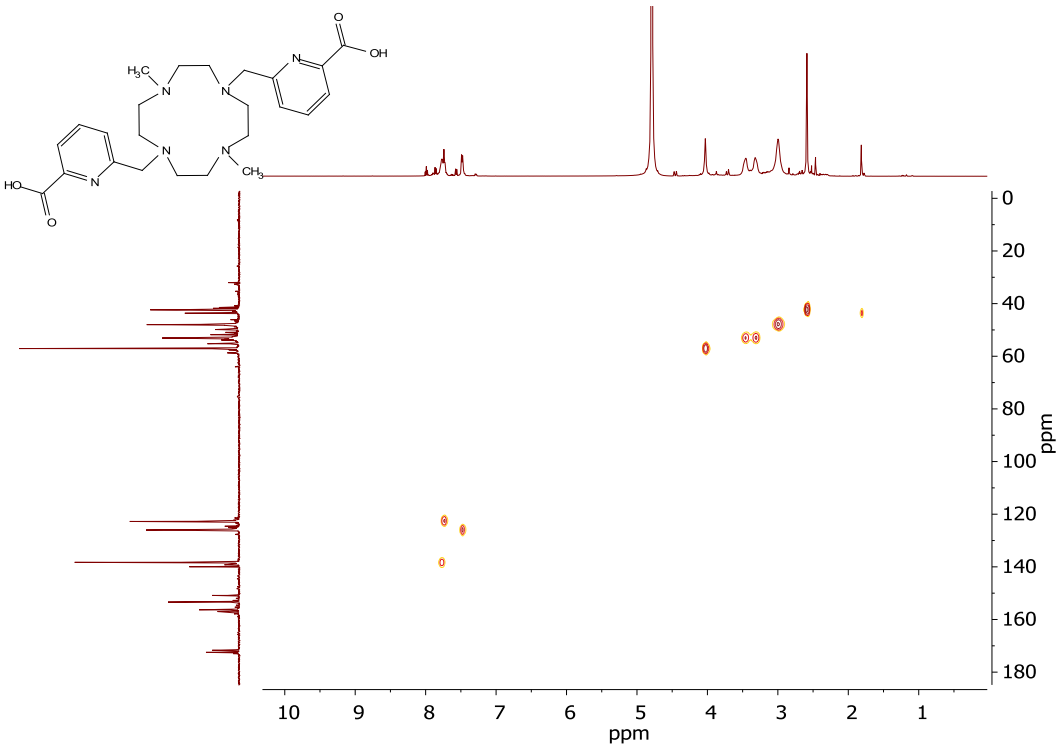
DEPT-RMN (D_2O, pD = 7,0) (δ/ppm)



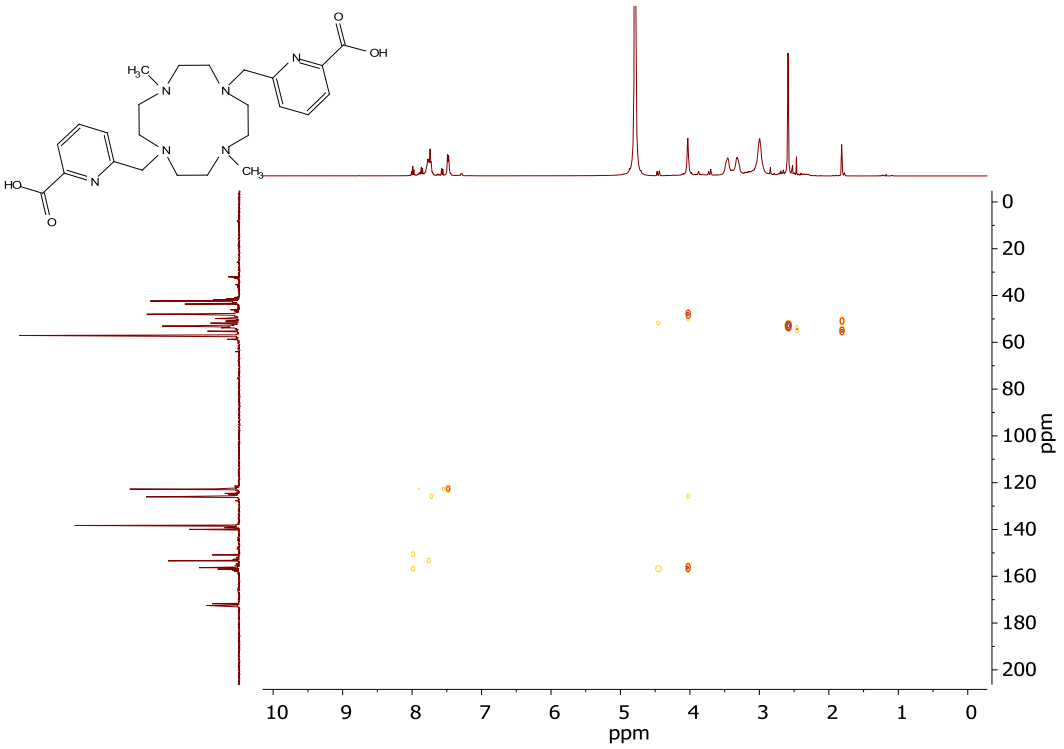
COSY-RMN (D_2O, pD = 7,0) (δ/ppm)



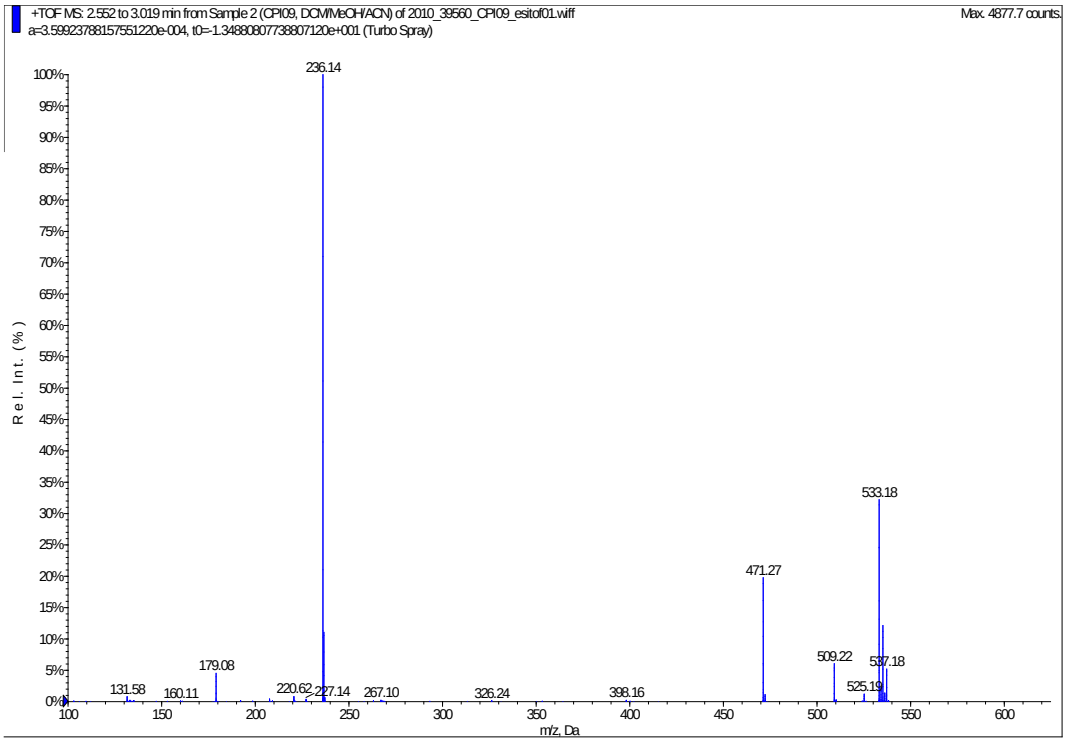
HSQC-RMN (D_2O, pD = 7,0) (δ/ppm)



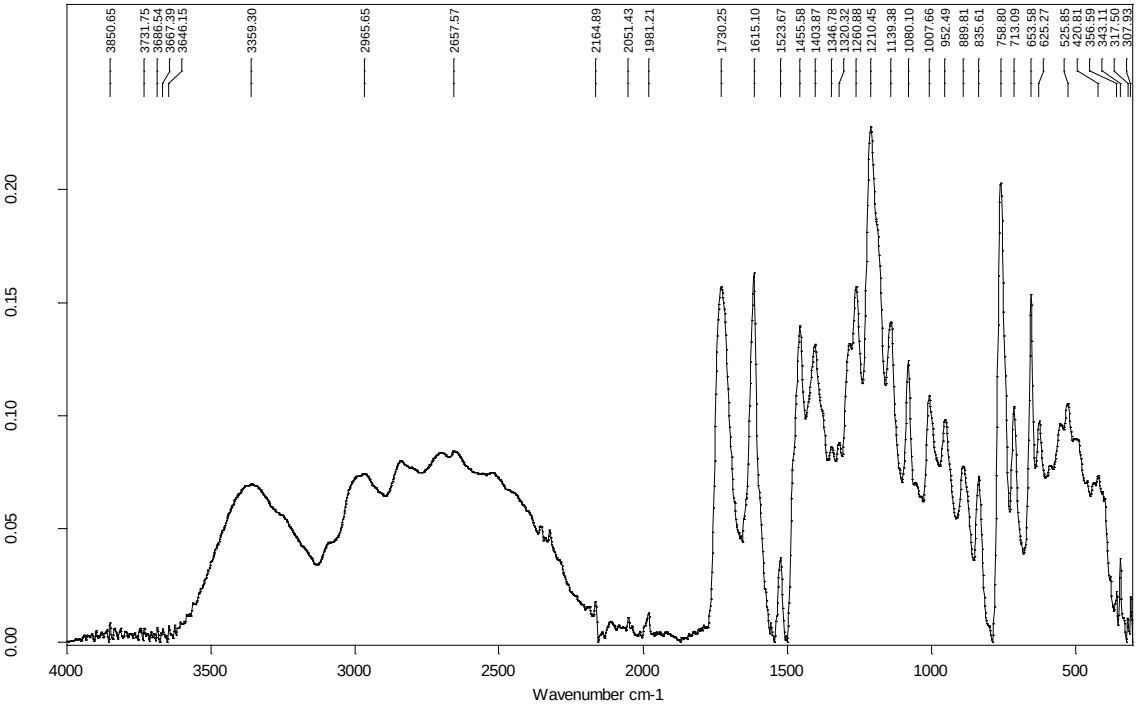
HMBC-RMN (D_2O, pD = 7,0) (δ/ppm)



Espectro de masas ESI+

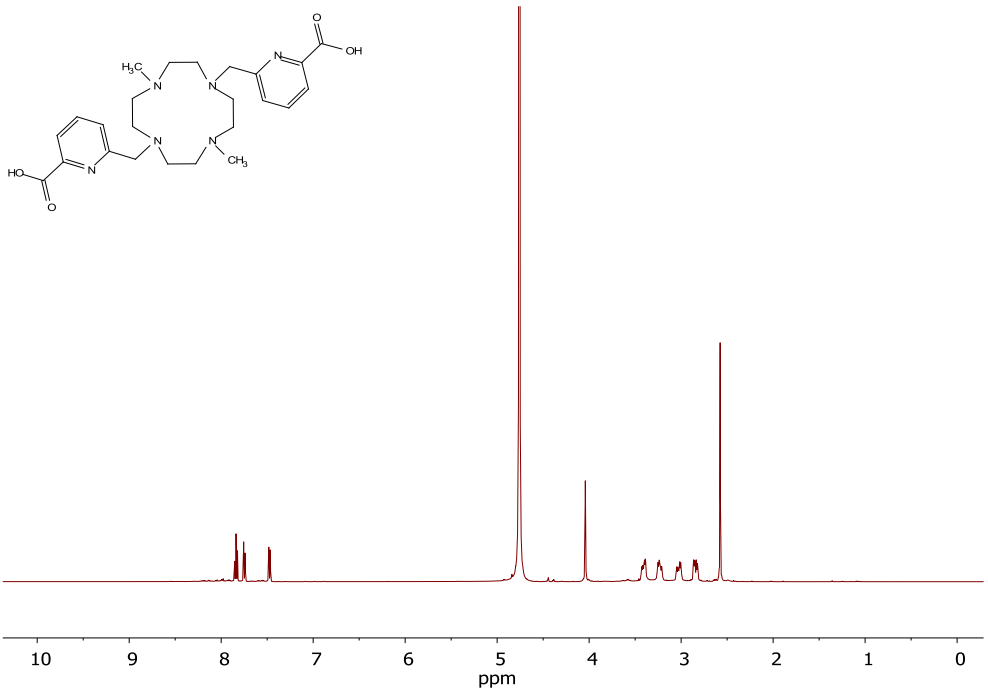


Espectro IR

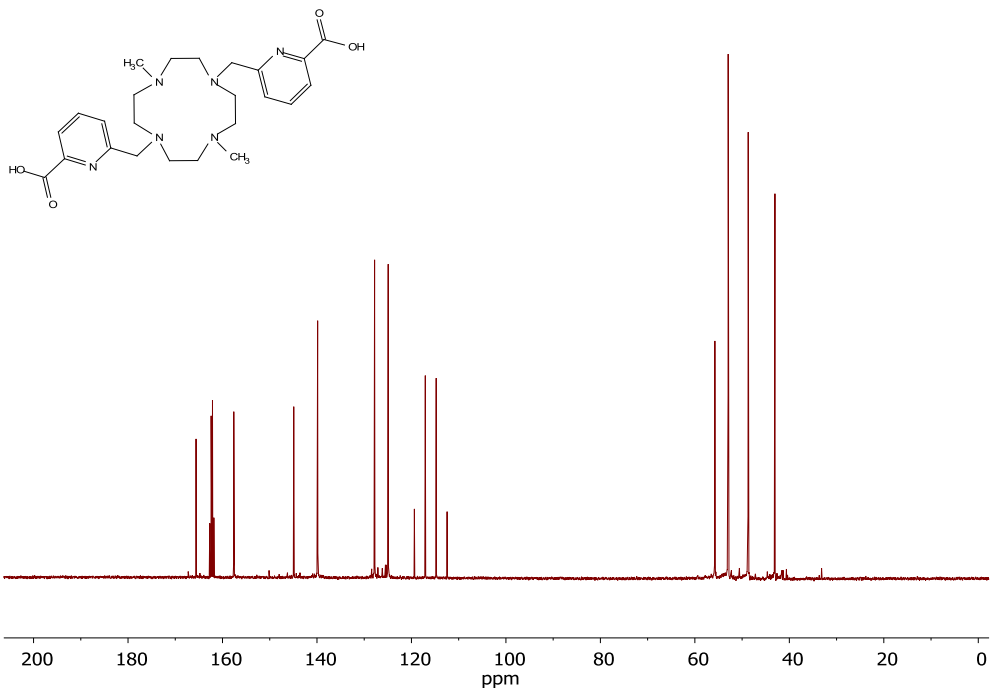


Ácido dimetil 6,6´ - ((4,10 – dimetil - 1,4,7,10 – tetraazaciclododecano - 1,7 - diil)bis(metilen))dipicolínico (**$H_2Me_2DODPA \cdot 11TFA$**)

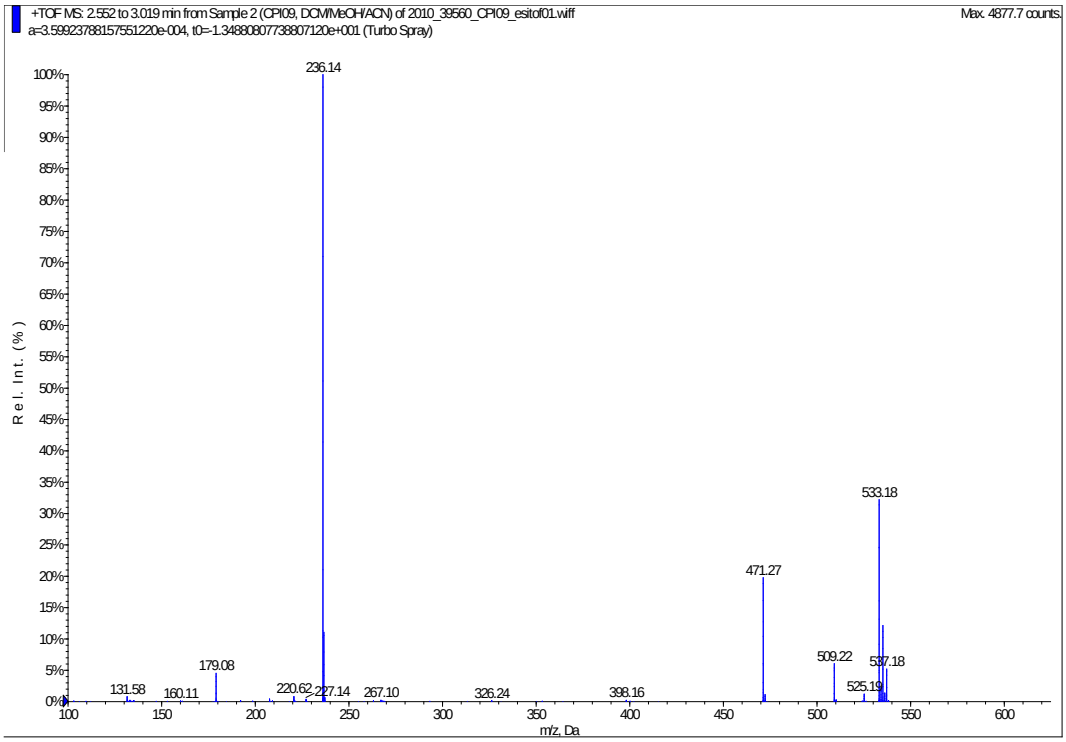
^{1}H-RMN (D_2O, 500 MHz, pD = 0,8) (δ/ppm)



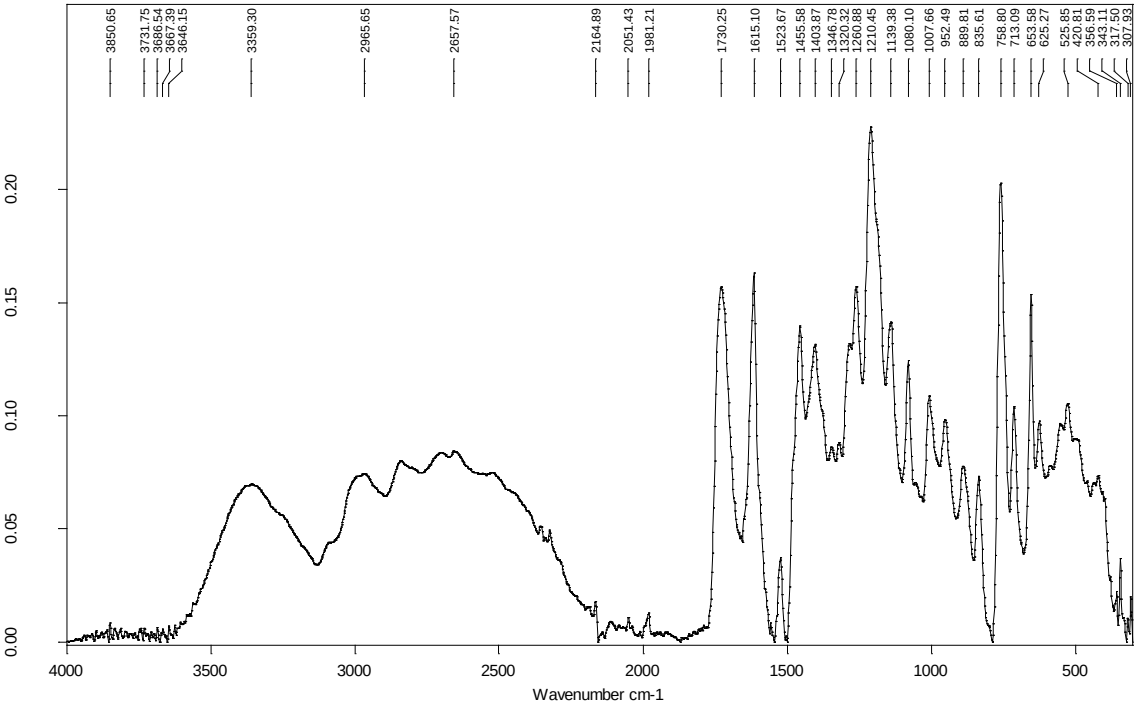
^{13}C-RMN (D_2O, 125,8 MHz, pD = 0,8) (δ/ppm)



Espectro de masas ESI+

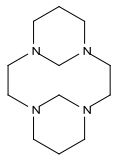


Espectro IR

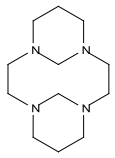


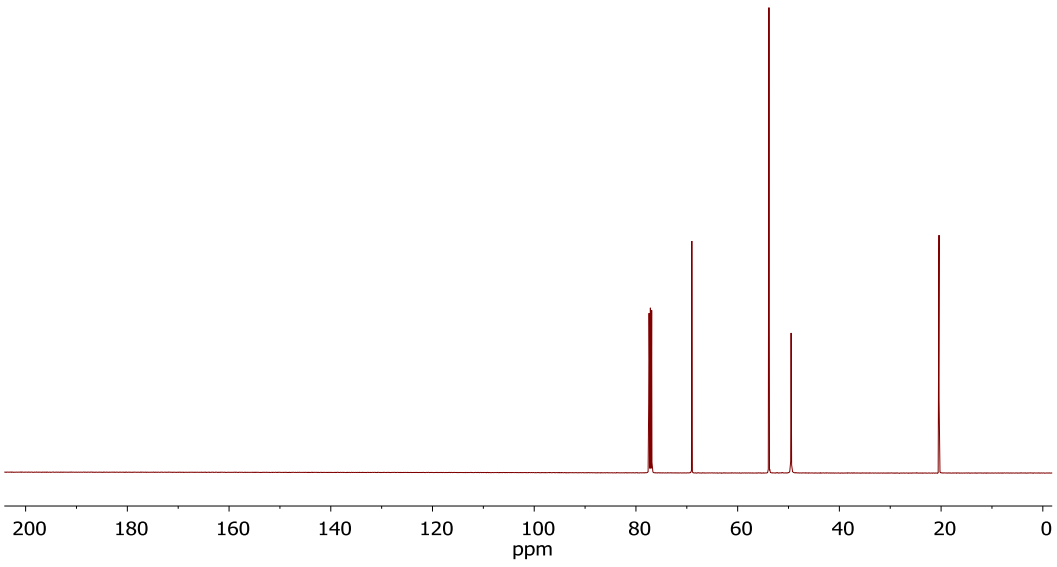
1,4,8,11-tetraazatriciclo[9.3.1.1^{4,8}]hexadecano (**20**)

^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)

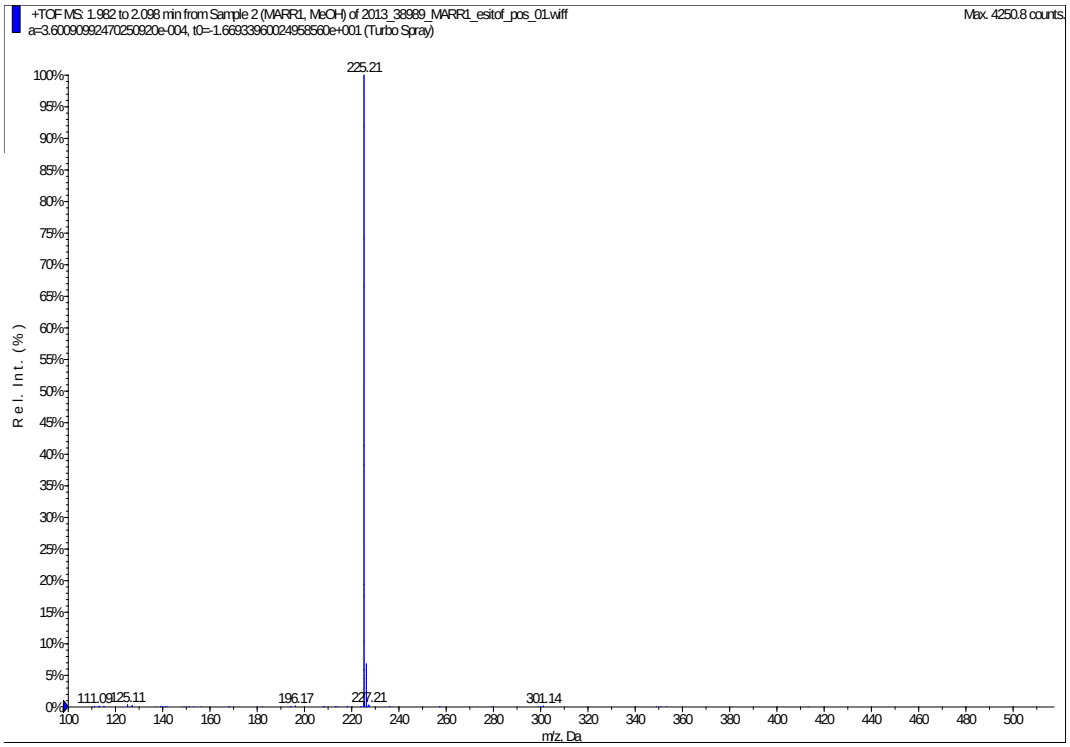


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

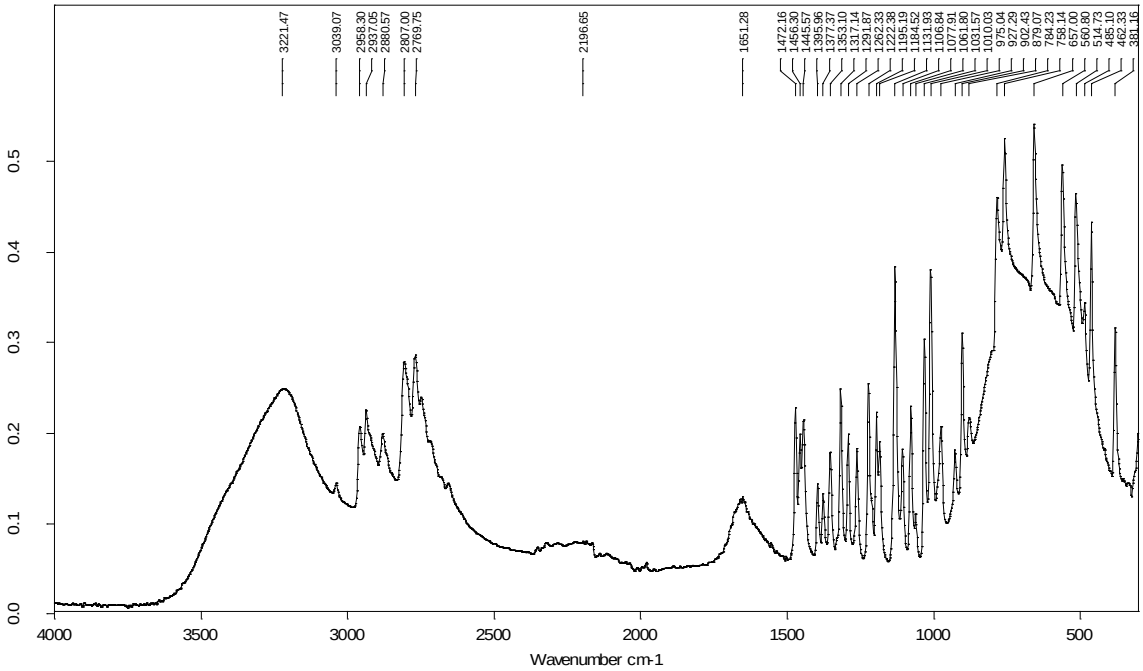




Espectro de masas ESI+

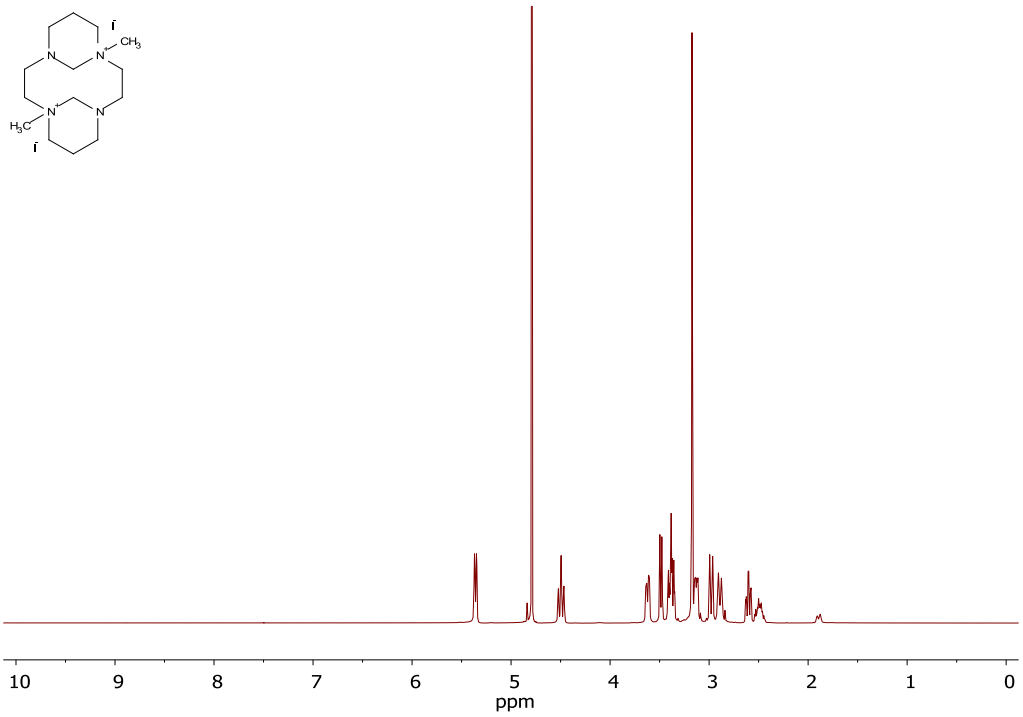


Espectro IR

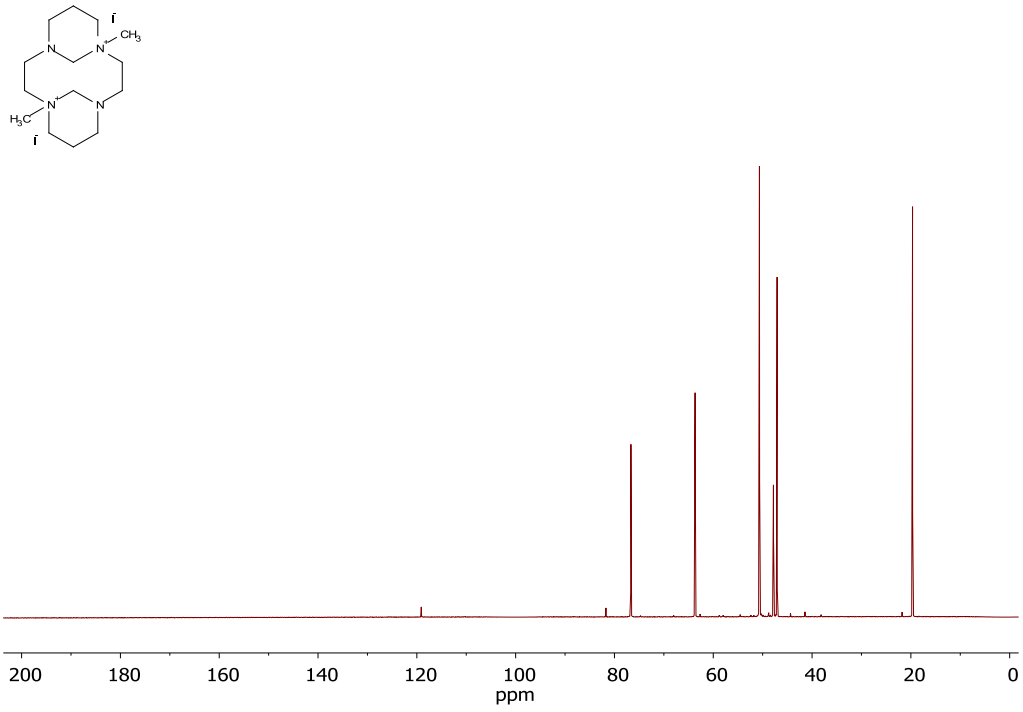


1,8-diyoduro de 1,8 – dimetil - 1,4,8,11 – tetraazatriciclo [9.3.1.1^{4,8}] hexadecano (**21**)

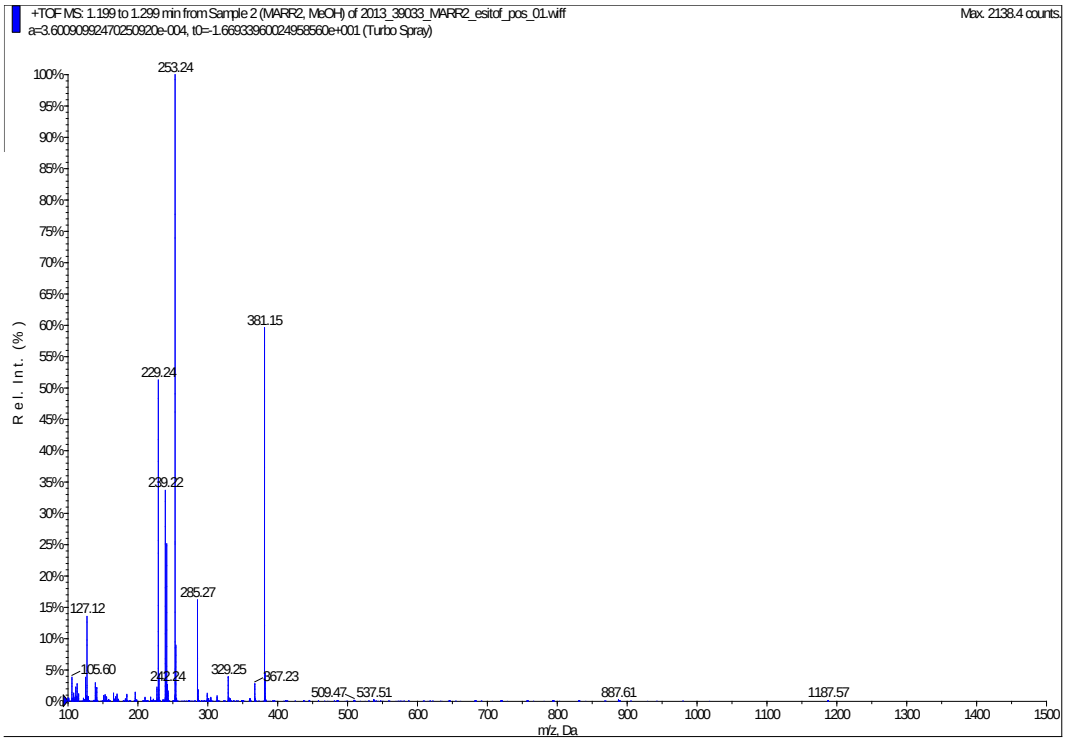
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



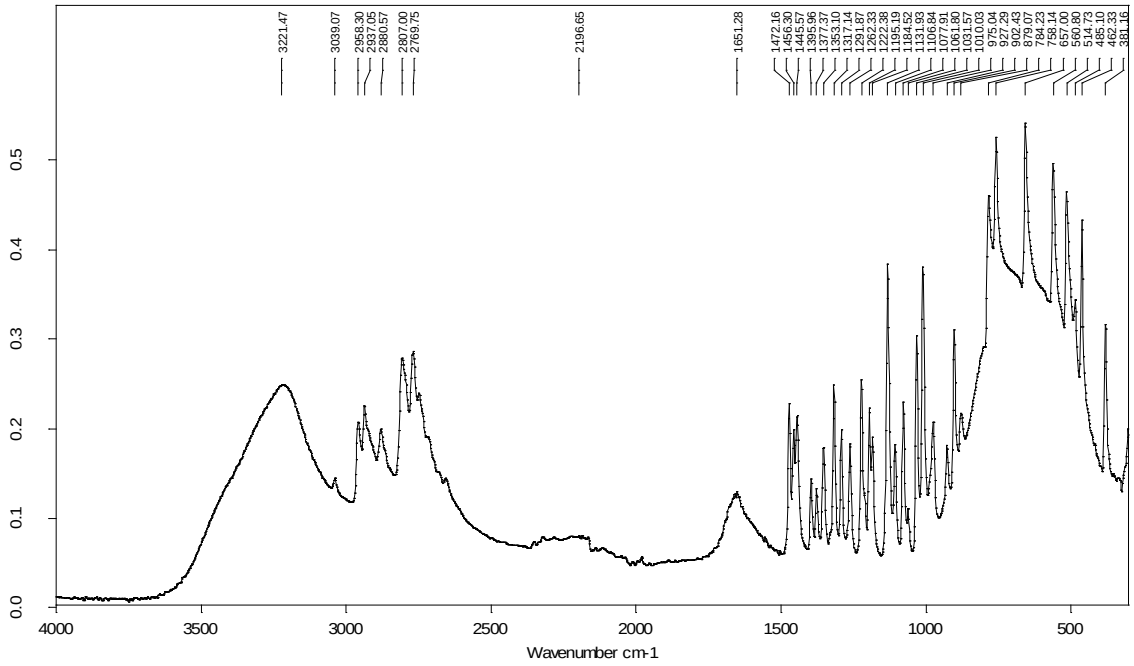
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



Espectro de masas ESI+

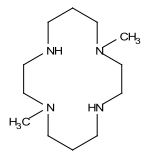


Espectro IR

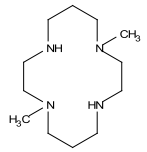


1,8-dimetil-1,4,8,11-tetraazaciclododecano (**22**)

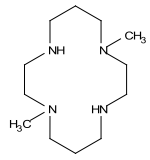
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



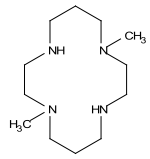
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



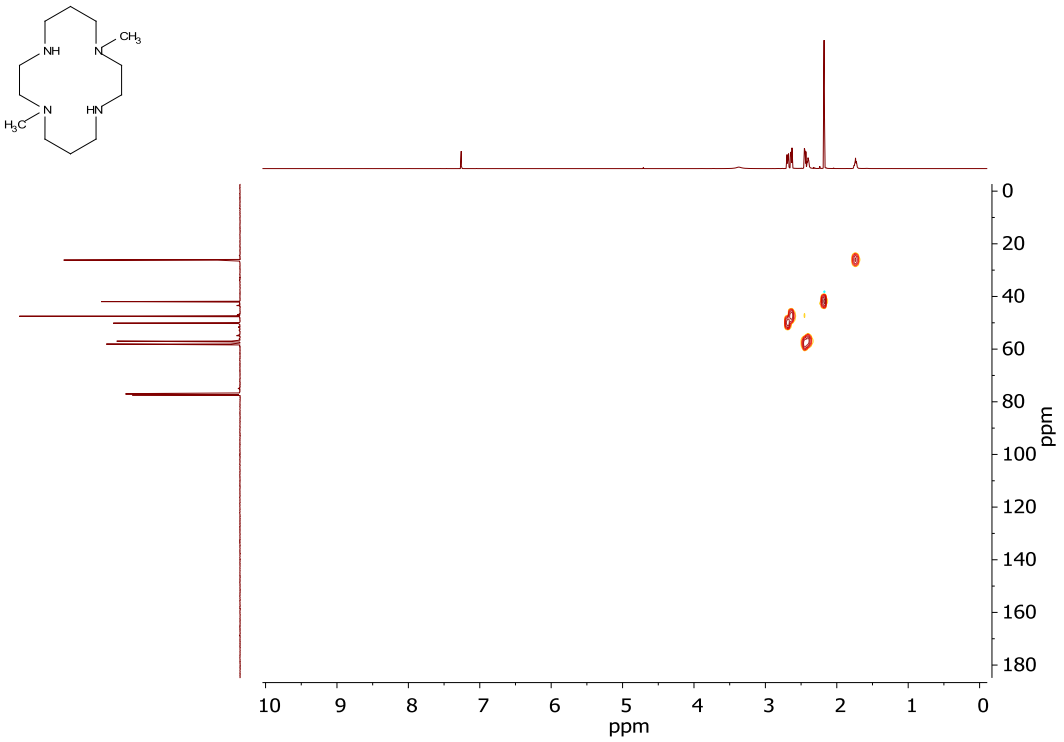
DEPT-RMN ($CDCl_3$) (δ/ppm)



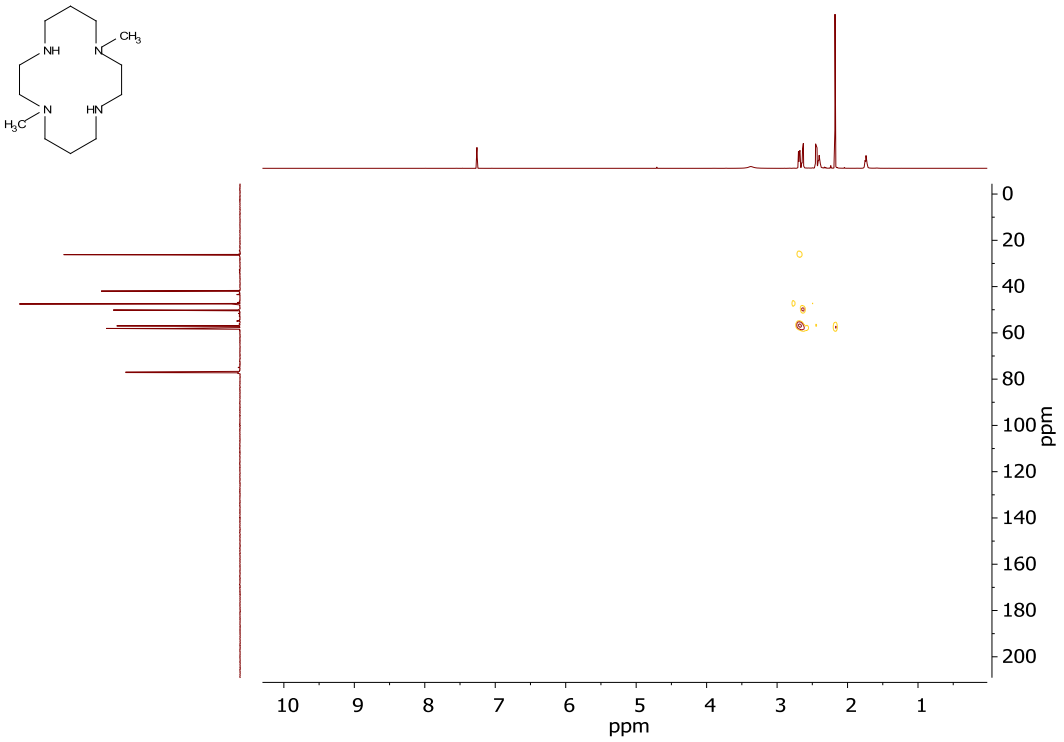
COSY-RMN ($CDCl_3$) (δ/ppm)



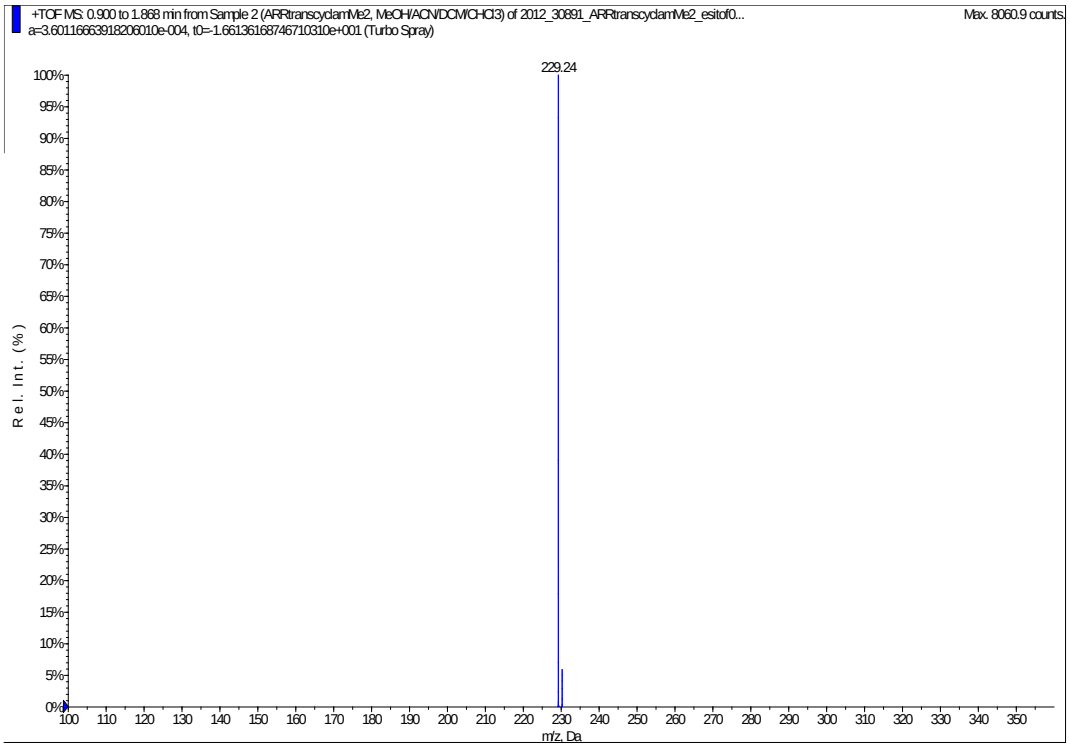
HSQC-RMN ($CDCl_3$) (δ/ppm)



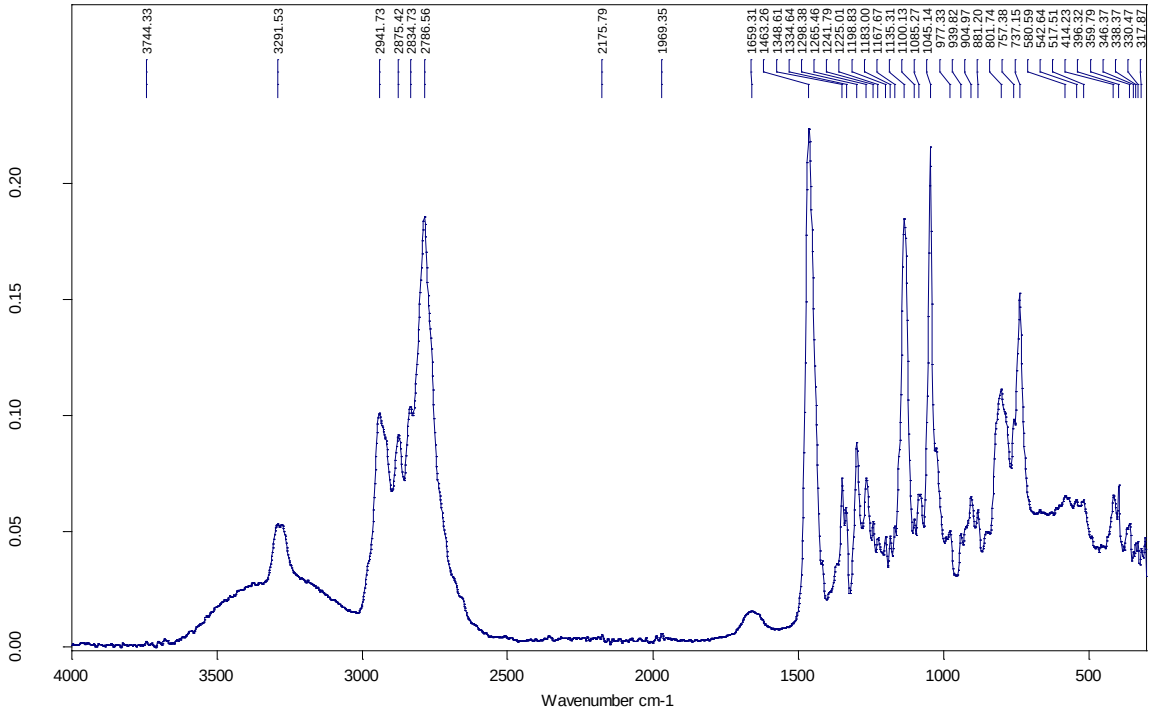
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

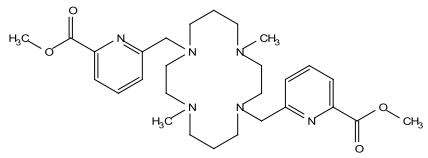


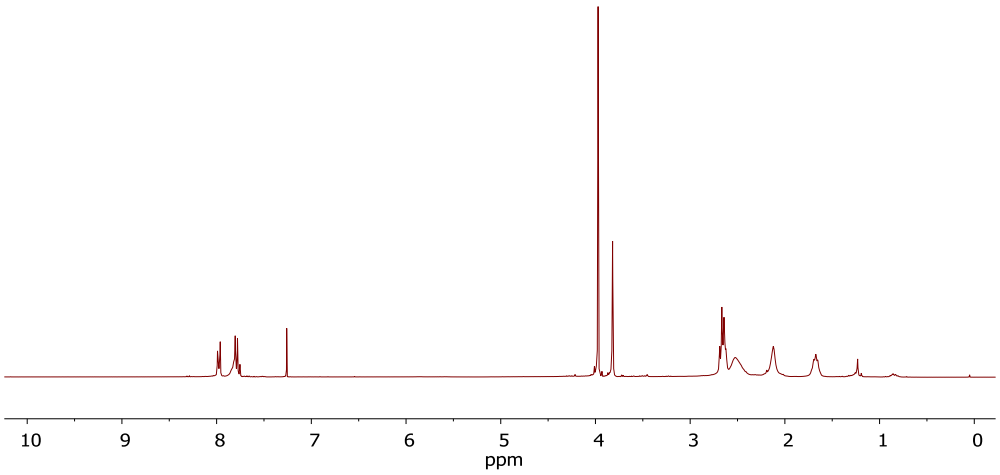
Espectro IR



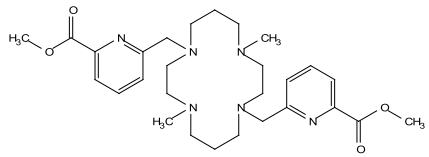
Dimetil 6,6' - ((4,11 – dimetil - 1,4,8,11 – tetraazaciclotetradecano - 1,8 - diil) bis(metilen))dipicolinato (**23**)

^{1}H-RMN ($CDCl_3$, 300 MHz) (δ/ppm)

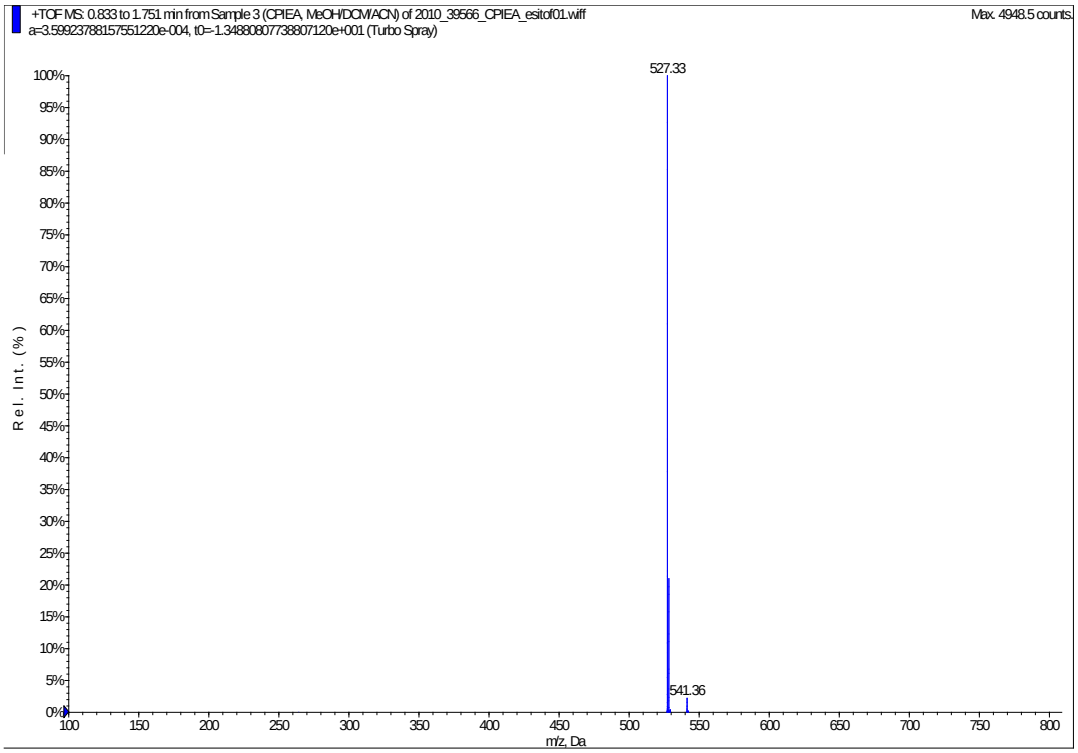




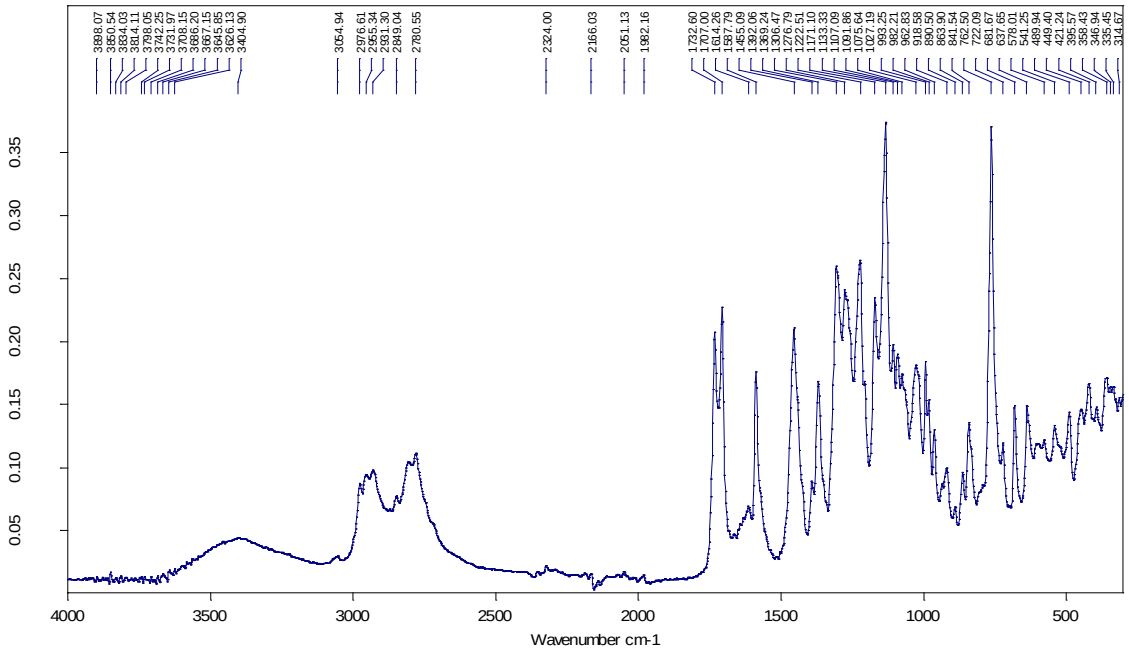
^{13}C-RMN ($CDCl_3$, 75,5 MHz) (δ/ppm)



Espectro de masas ESI+

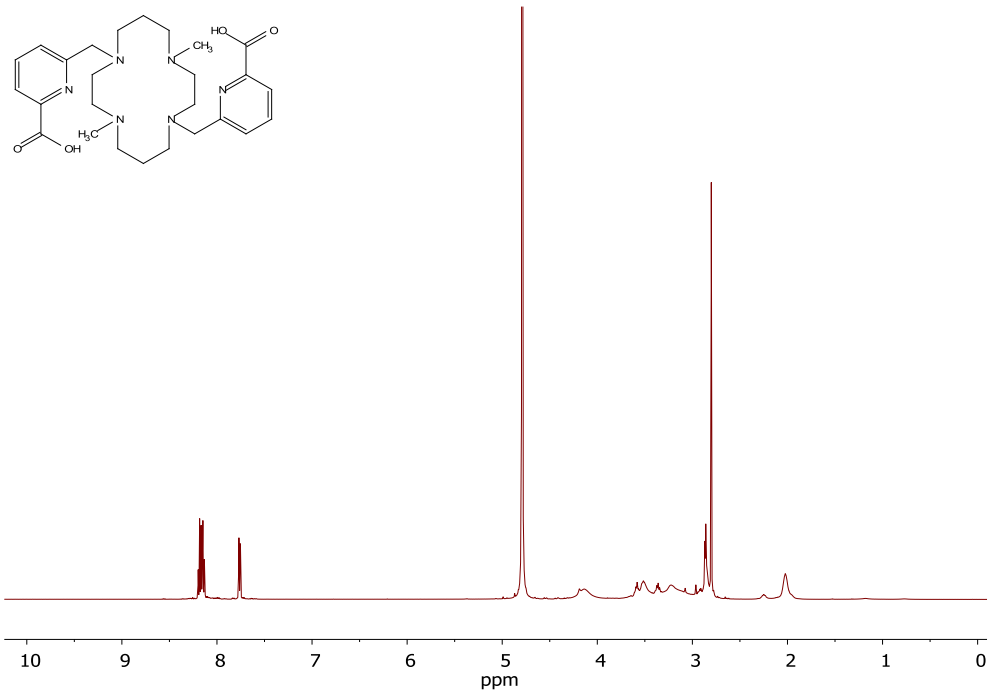


Espectro IR

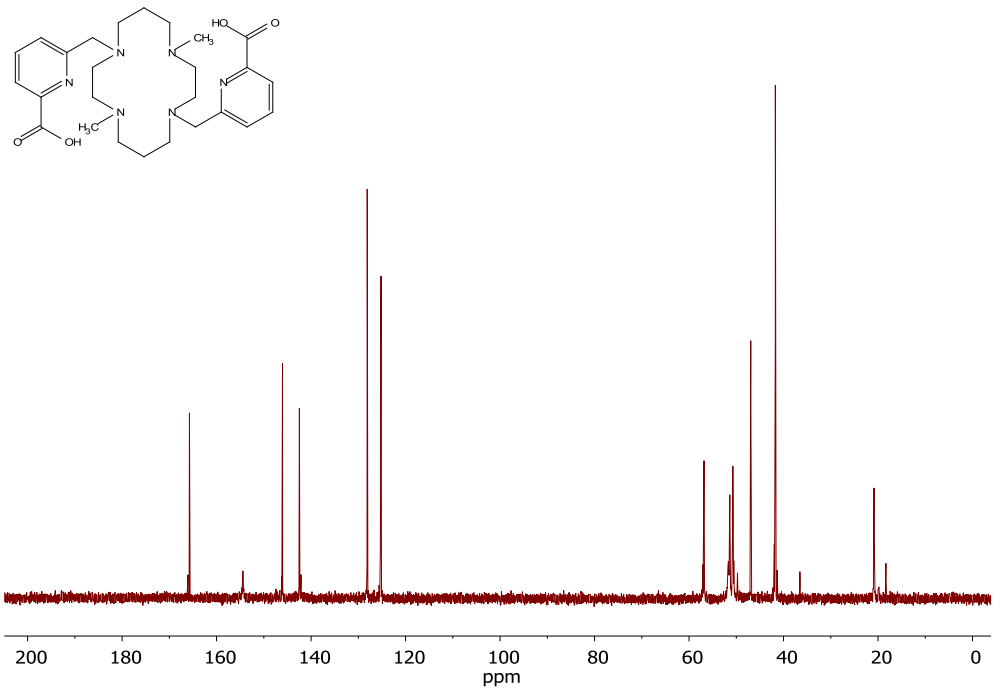


Ácido 6,6' - ((4,11 – dimetil - 1,4,8,11 – tetraazaciclotetradecano - 1,8 - diil) bis(metilen)) dipicolínico ($H_2Me_2tedpa \cdot 5HCl \cdot 3H_2O$)

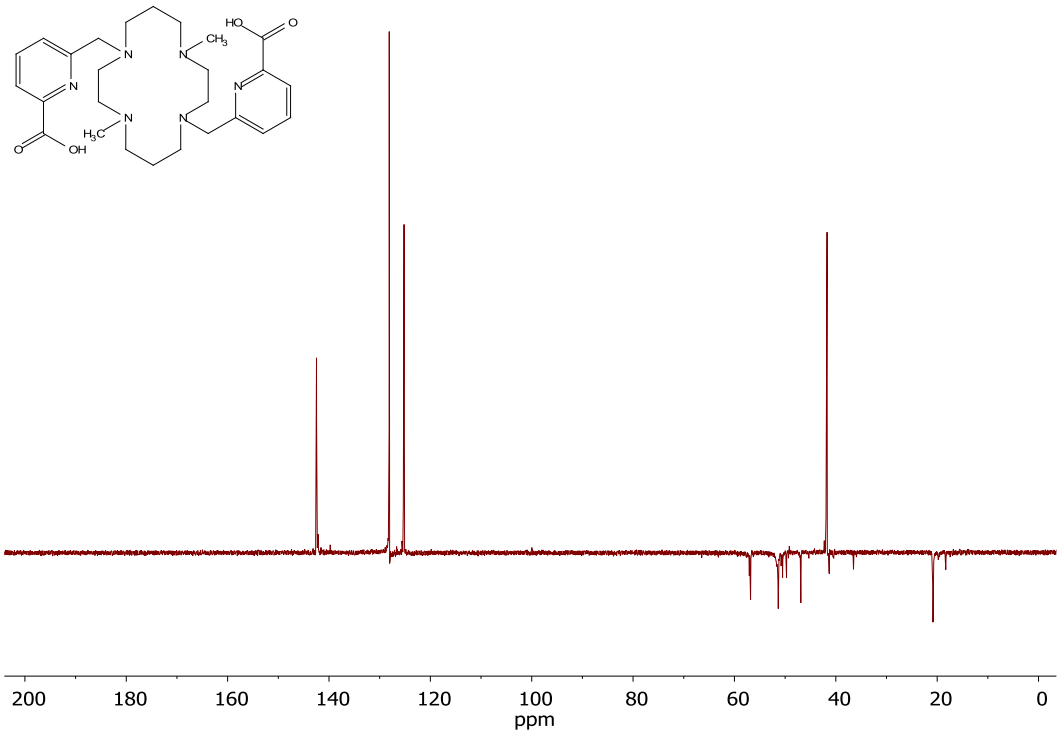
^{1}H-RMN (D_2O, 500 MHz, pD = 0,7) (δ/ppm)



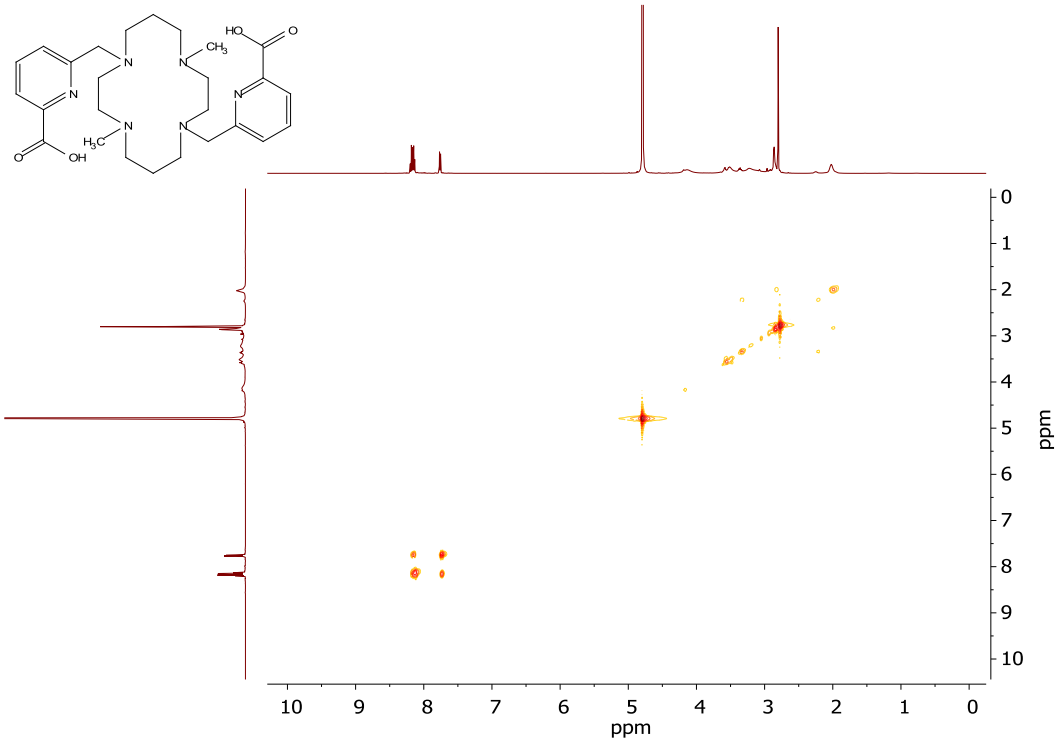
^{13}C-RMN ($CDCl_3$, 125,8 MHz, pD = 0,7) (δ/ppm)



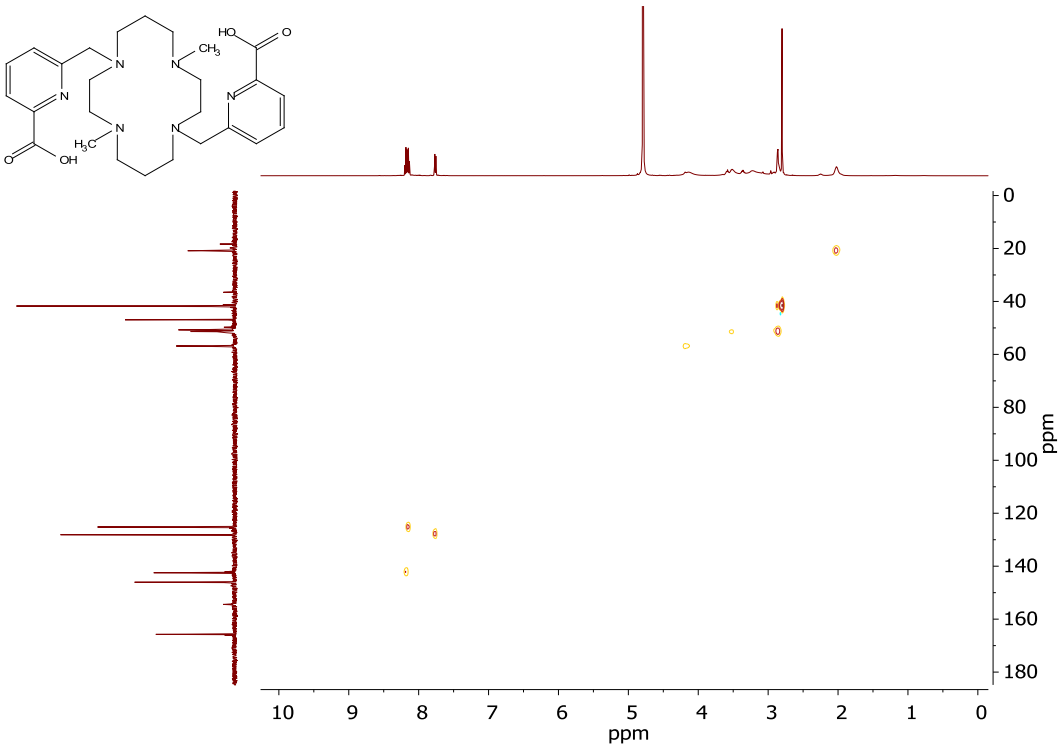
DEPT-RMN (D_2O, pD = 0,7) (δ/ppm)



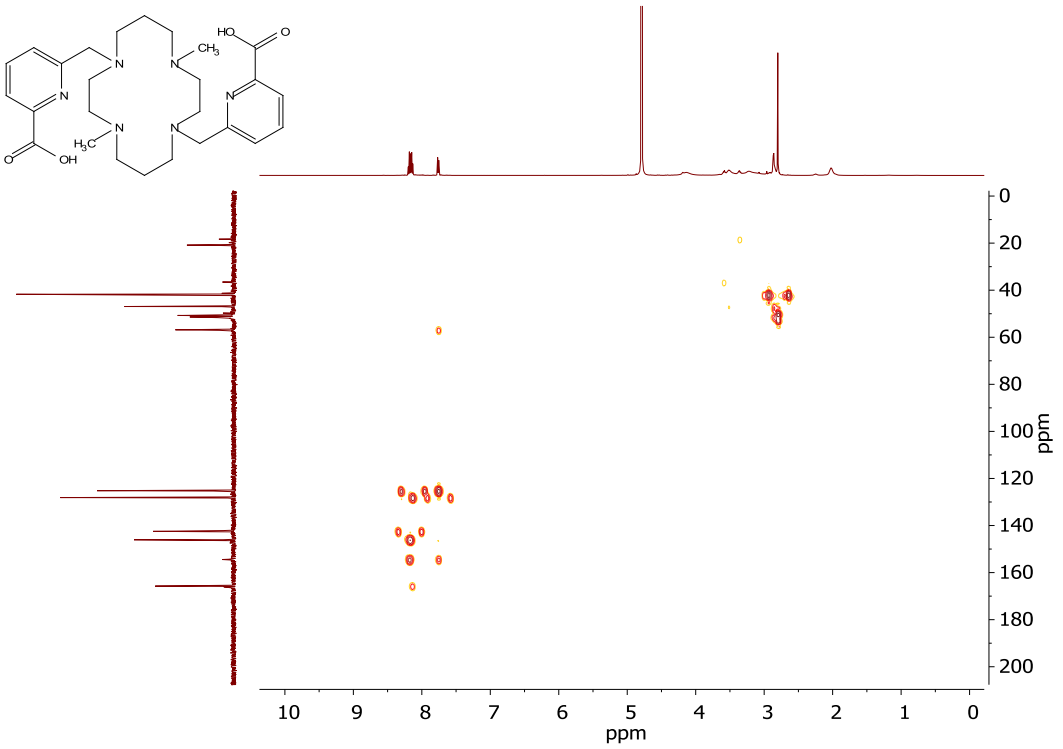
COSY-RMN (D_2O, pD = 0,7) (δ/ppm)



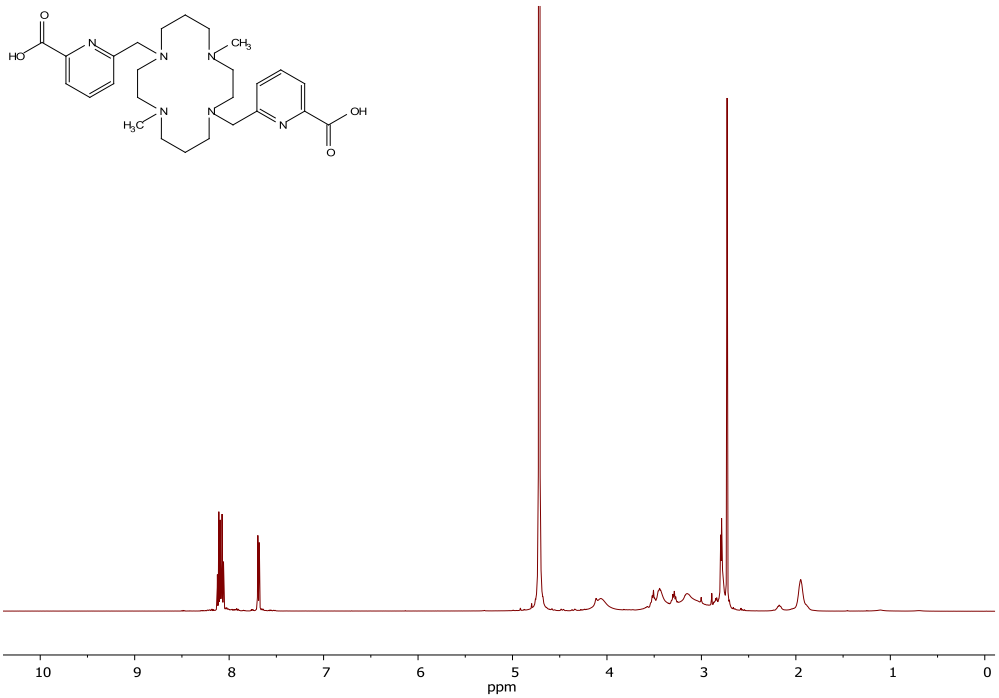
HSQC-RMN (D_2O, pD = 0,7) (δ/ppm)



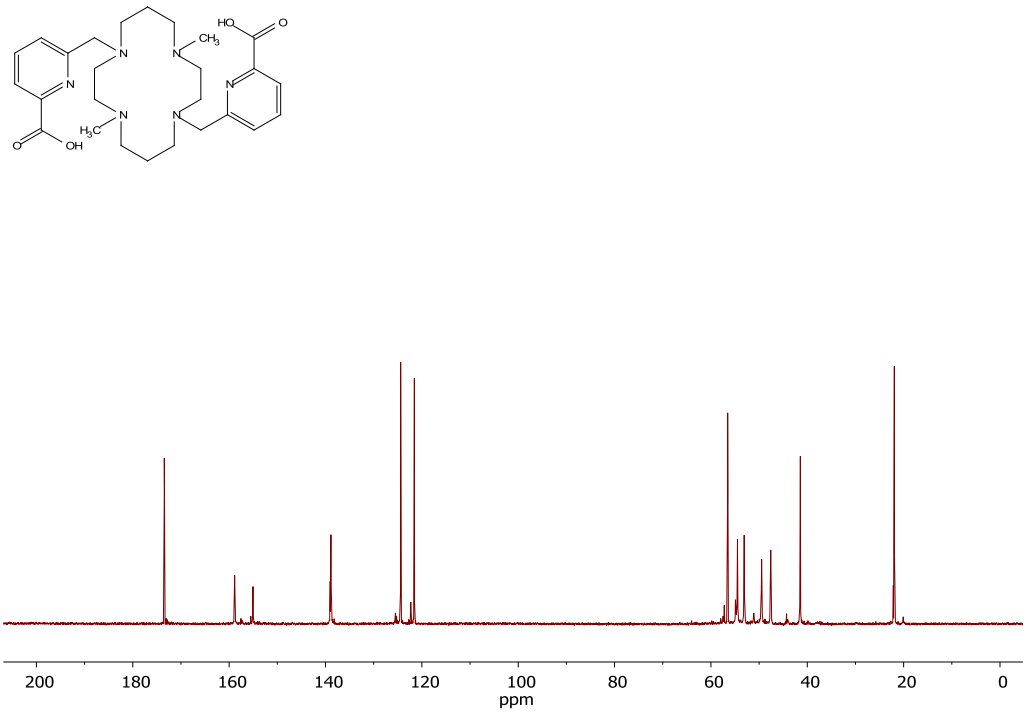
HMBC-RMN (D_2O, pD = 0,7) (δ/ppm)



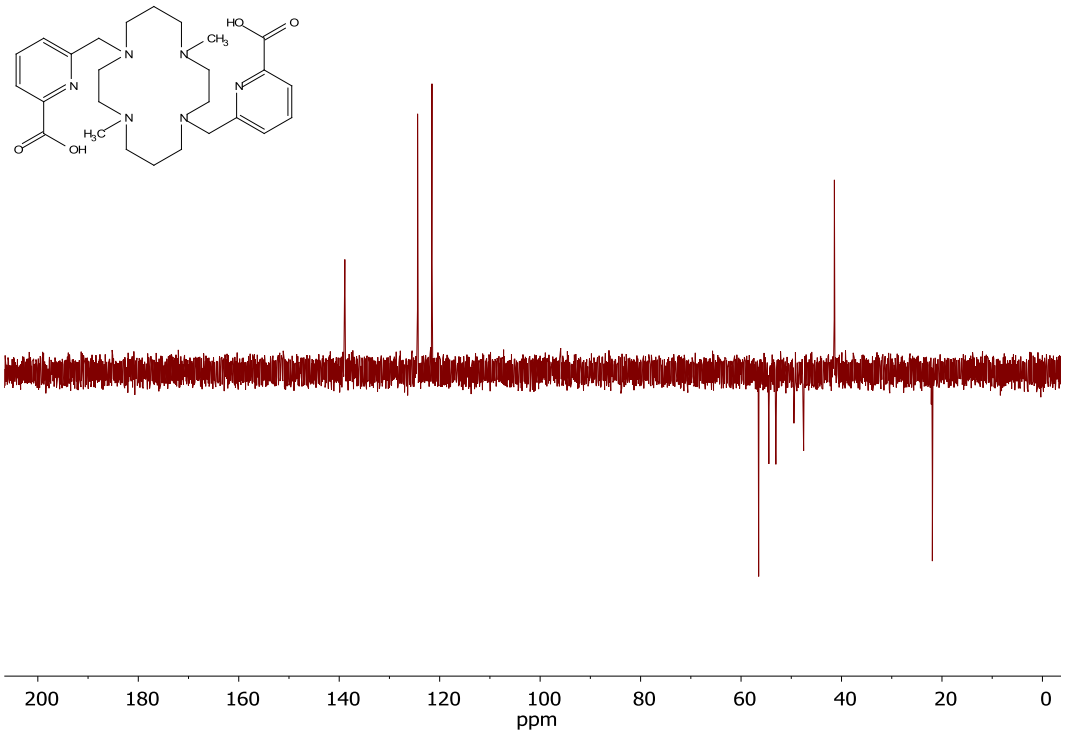
^{1}H-RMN (D_2O, 500 MHz, pD = 7,1) (δ/ppm)



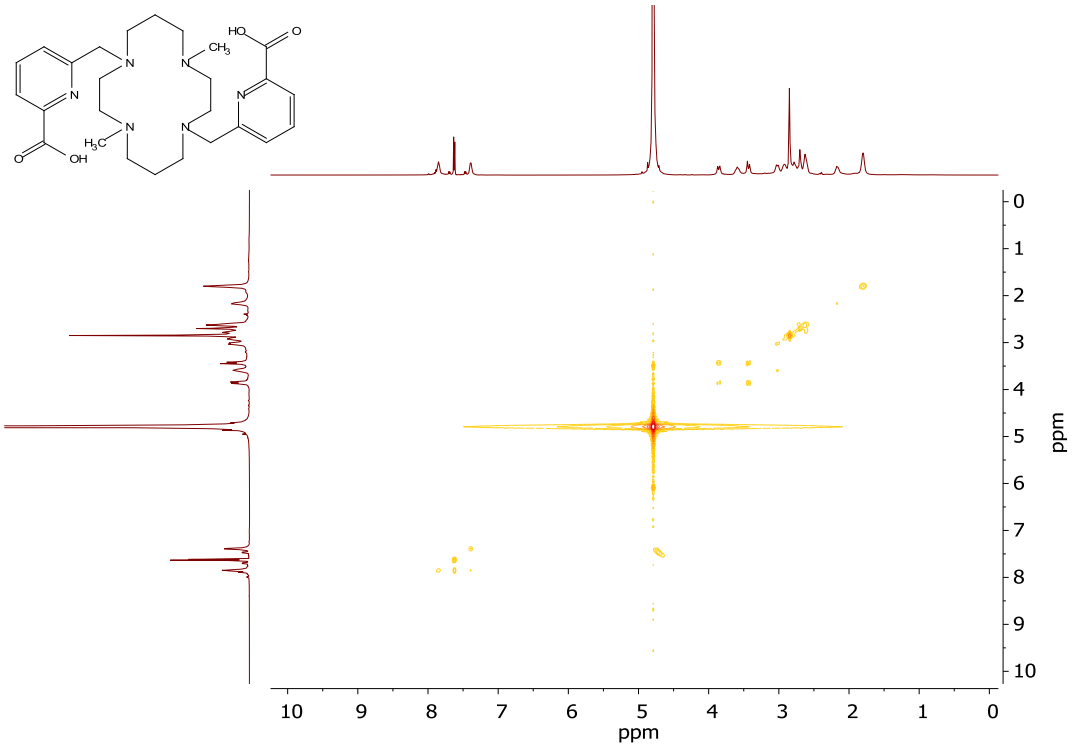
^{13}C-RMN (D_2O, 125,8 MHz, pD = 7,1) (δ/ppm)



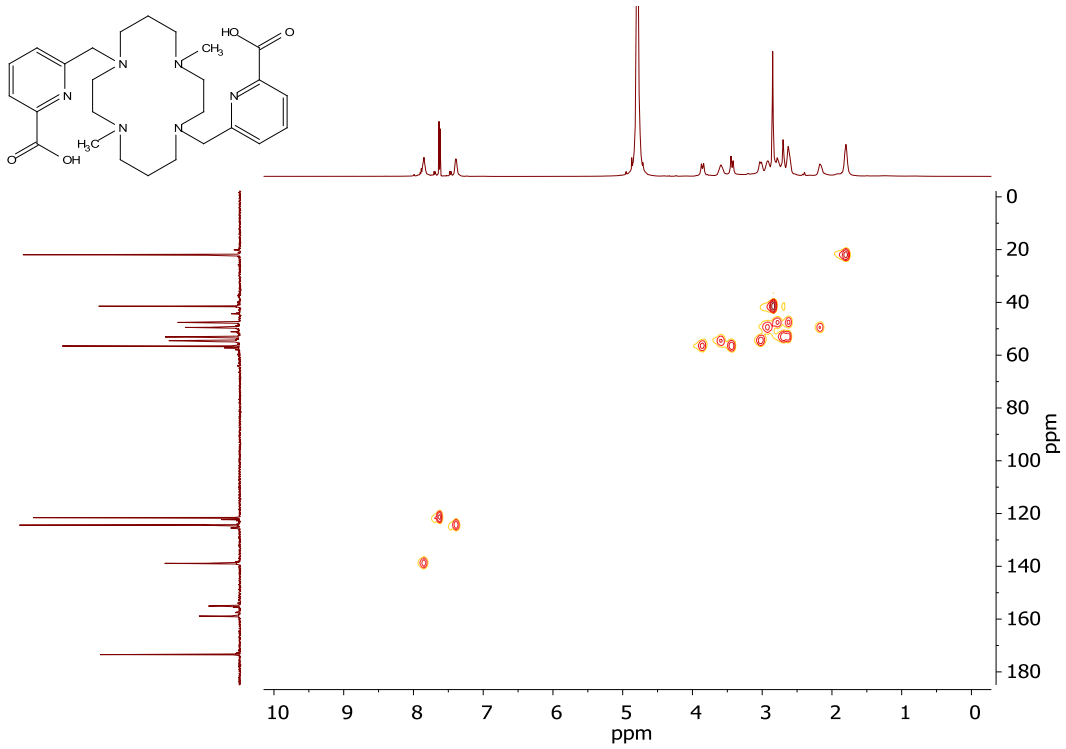
DEPT-RMN (D_2O, pD = 7,1) (δ/ppm)



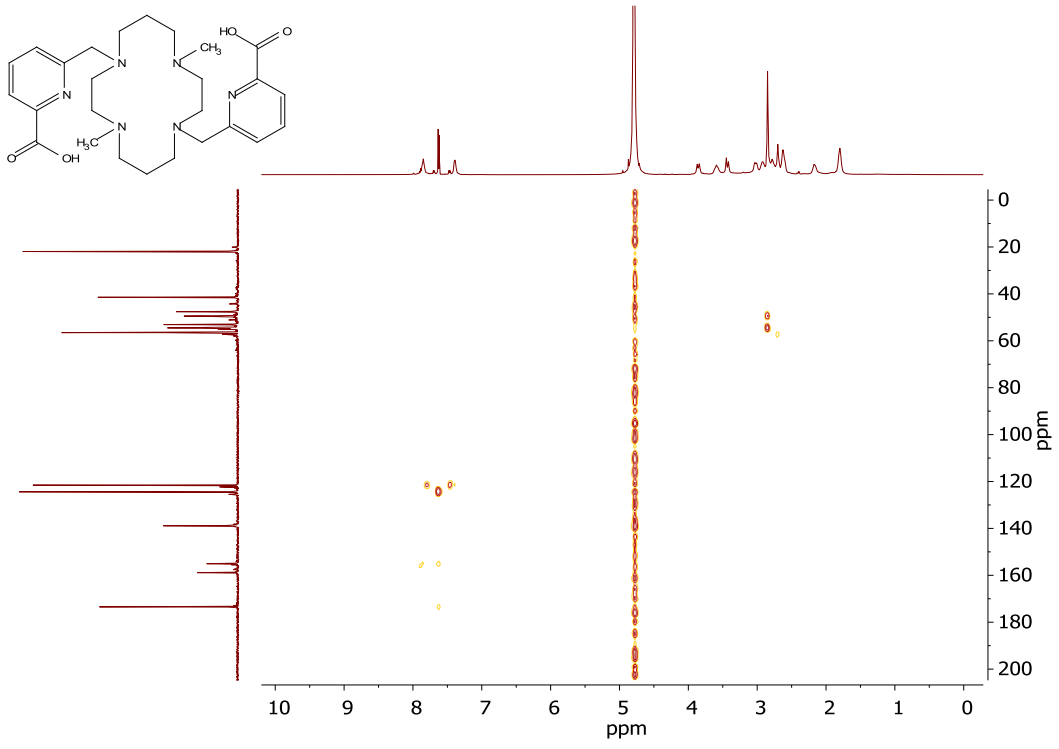
COSY-RMN (D_2O, pD = 7,1) (δ/ppm)



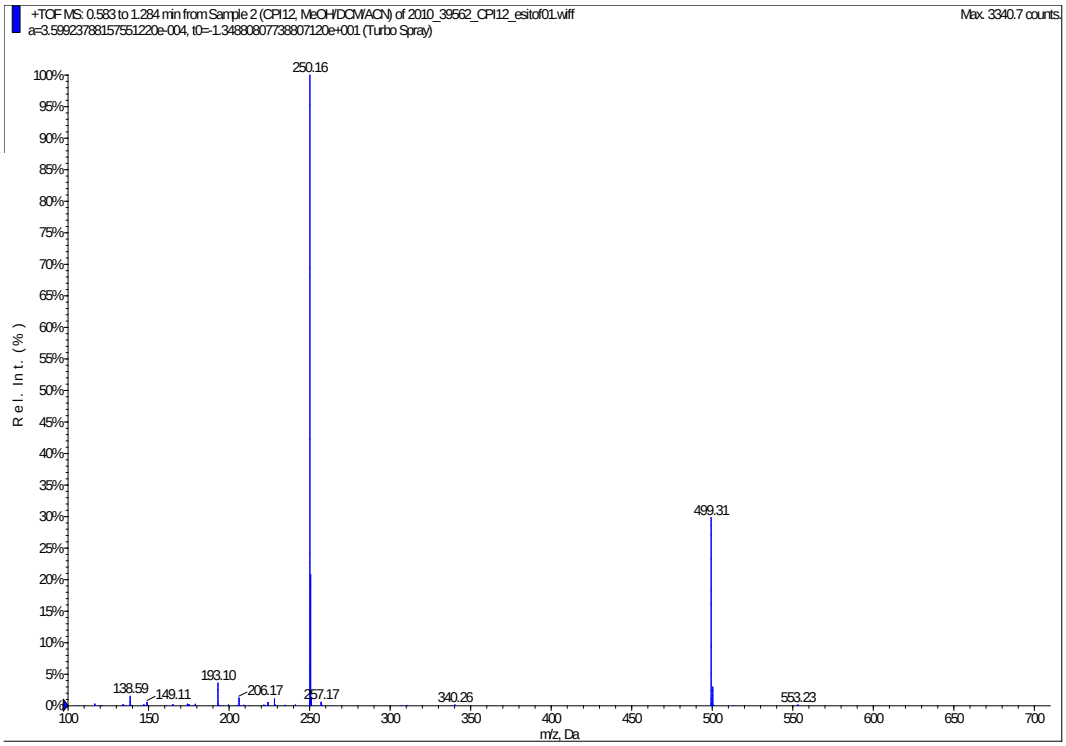
HSQC-RMN (D_2O, pD = 7,1) (δ/ppm)



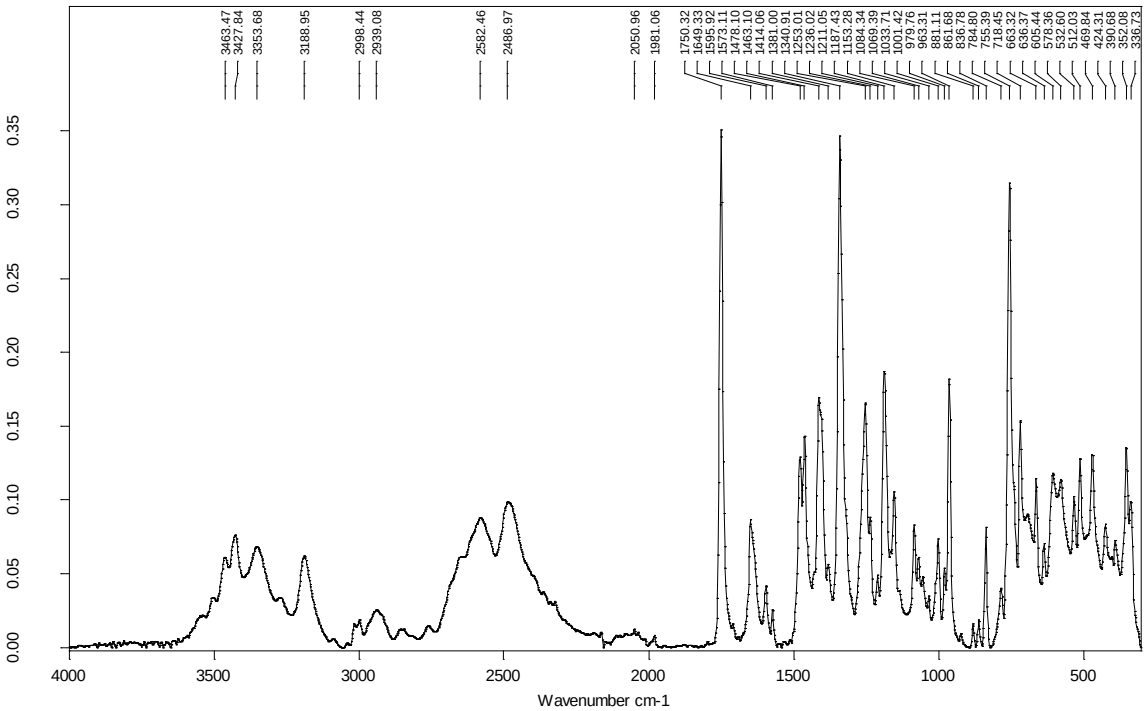
HMBC-RMN (D_2O, pD = 7,1) (δ/ppm)



Espectro de masas ESI+

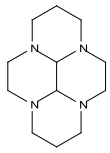


Espectro IR

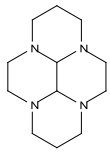


Decahidro - 1H,6H - 3a,5a,8a,10a - tetraazapireno - ciclam-glioxal – (**24**)

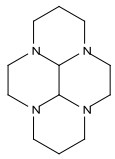
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



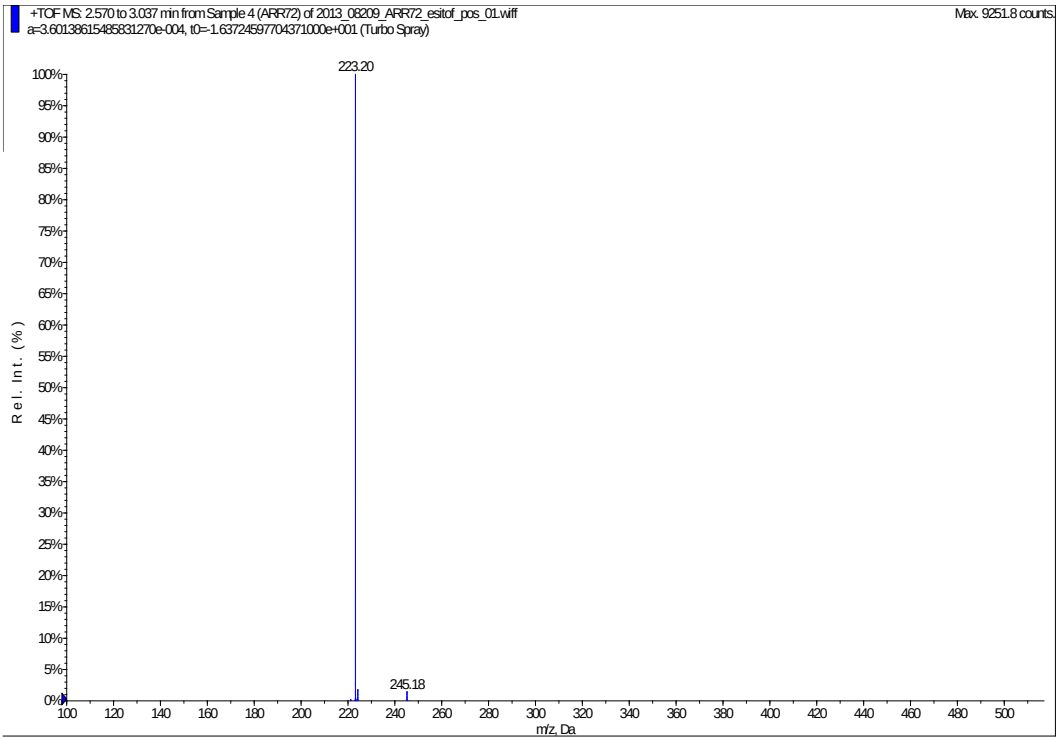
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



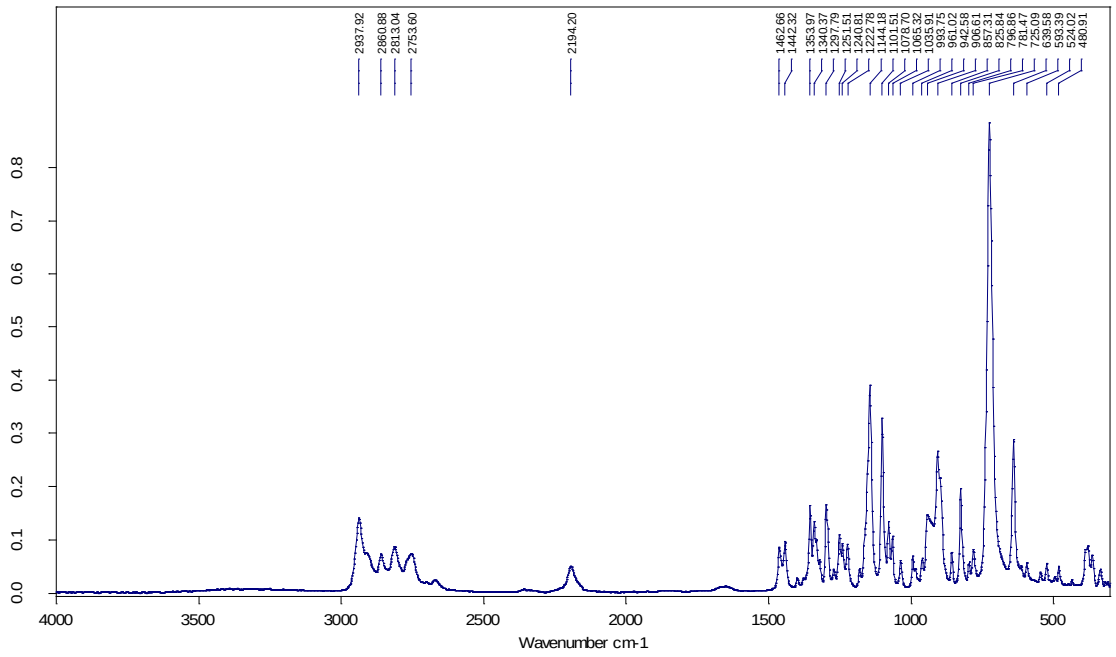
DEPT-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



Espectro de masas ESI^+

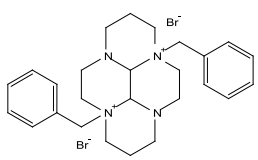


Espectro IR

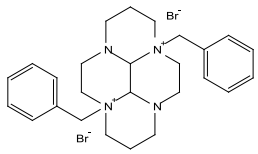

2937.92
2860.88
2813.04
2753.60
2194.20
1462.66
1442.32
1353.97
1340.37
1297.79
1251.51
1240.81
1222.78
1144.18
1101.51
1078.70
1065.32
1035.91
993.75
961.02
947.58
906.61
857.31
825.84
796.86
781.47
725.08
635.58
593.39
524.02
480.91
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

3a,8a - dibromuro de 3a,8a – dibenciltetradecahidro - 3a,5a,8a,10a – tetraazapireno (**25**)

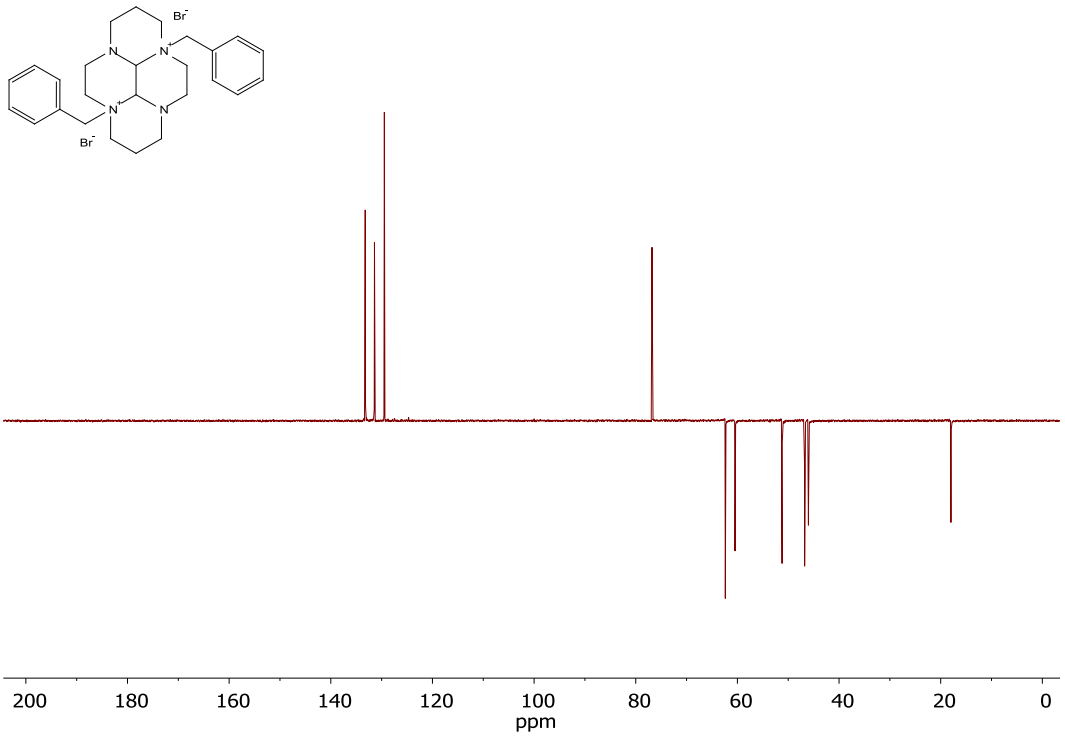
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



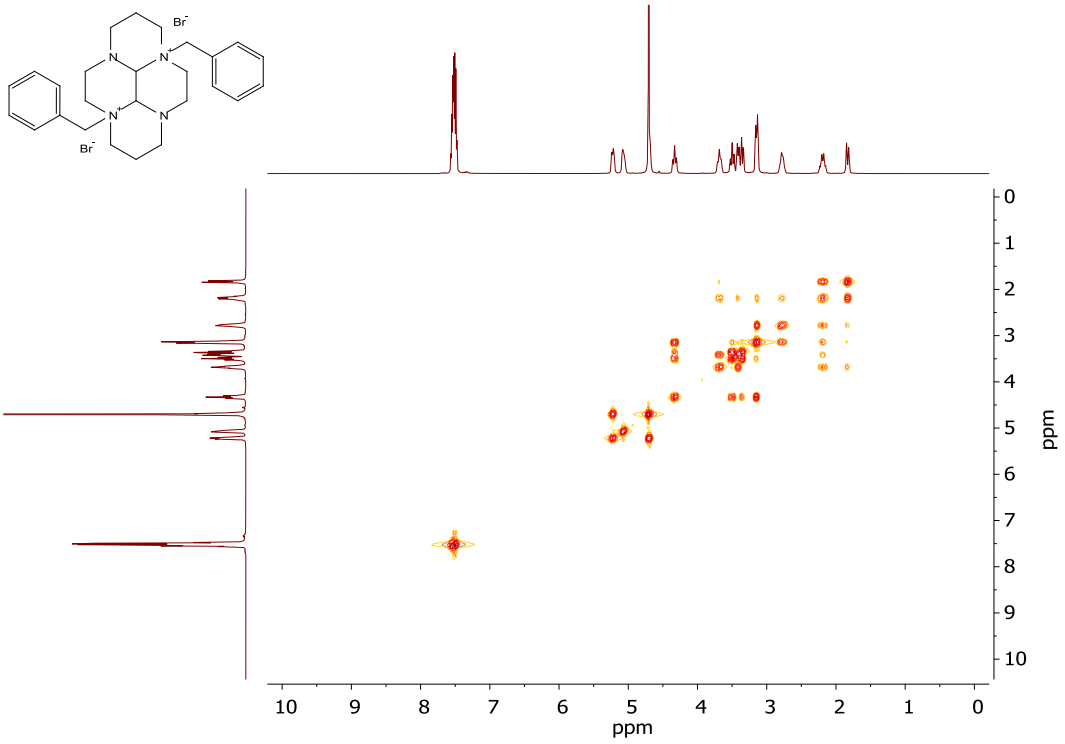
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



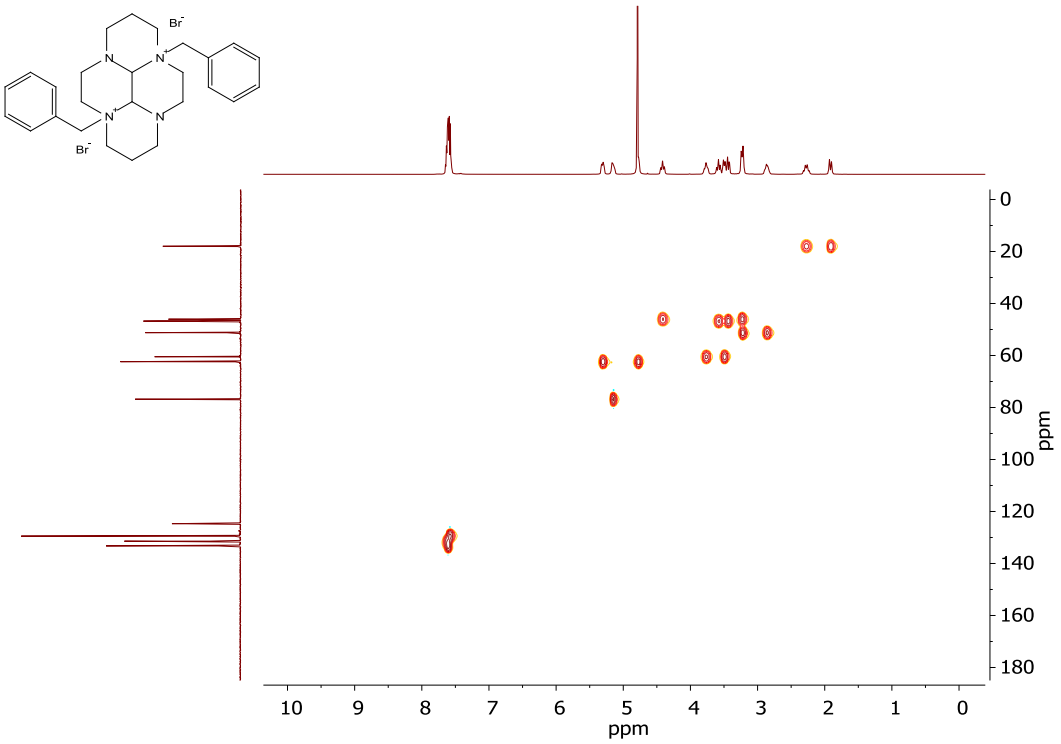
DEPT-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



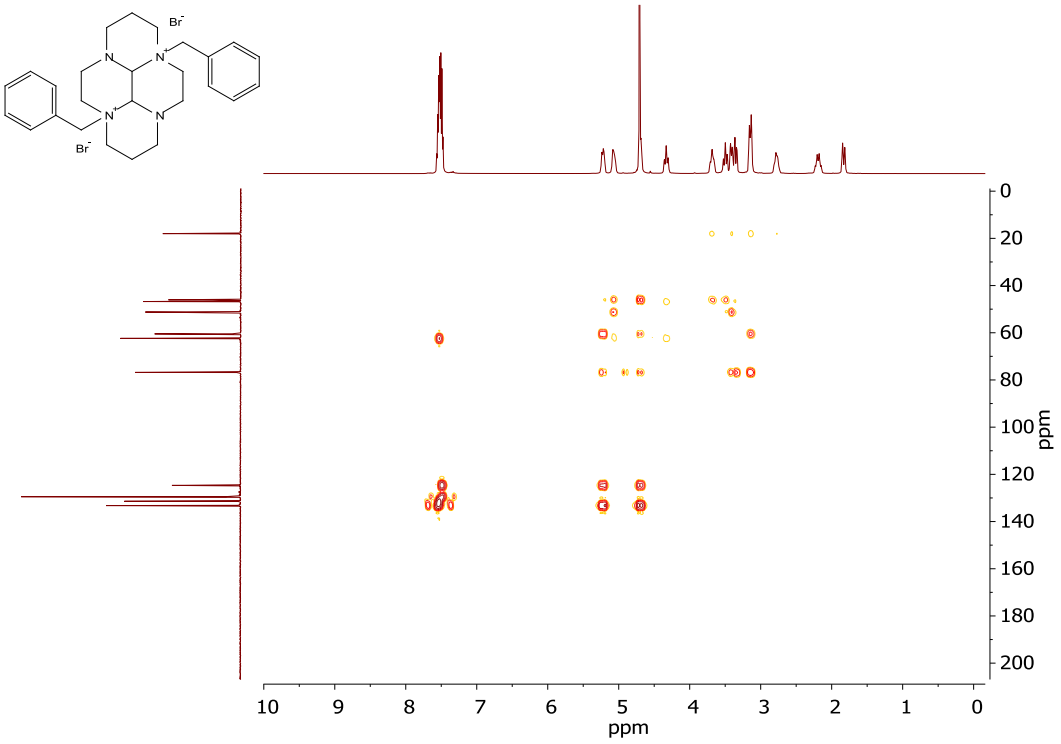
COSY-RMN (D_2O) (δ/ppm)



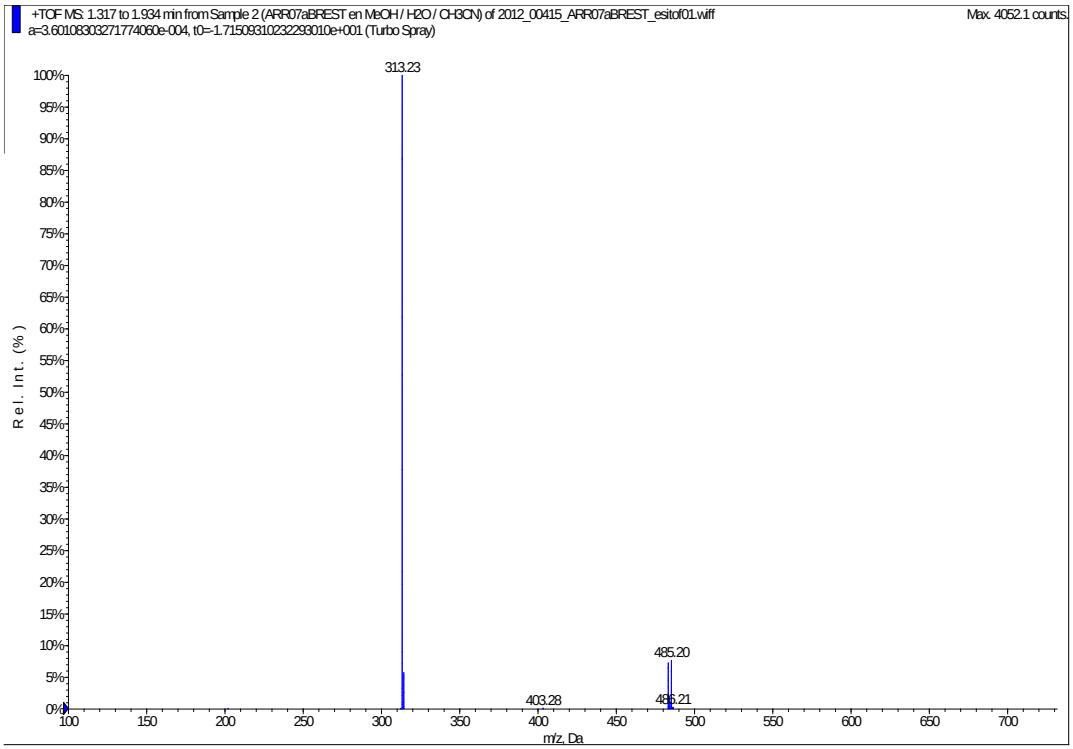
HSQC-RMN (D_2O) (δ/ppm)



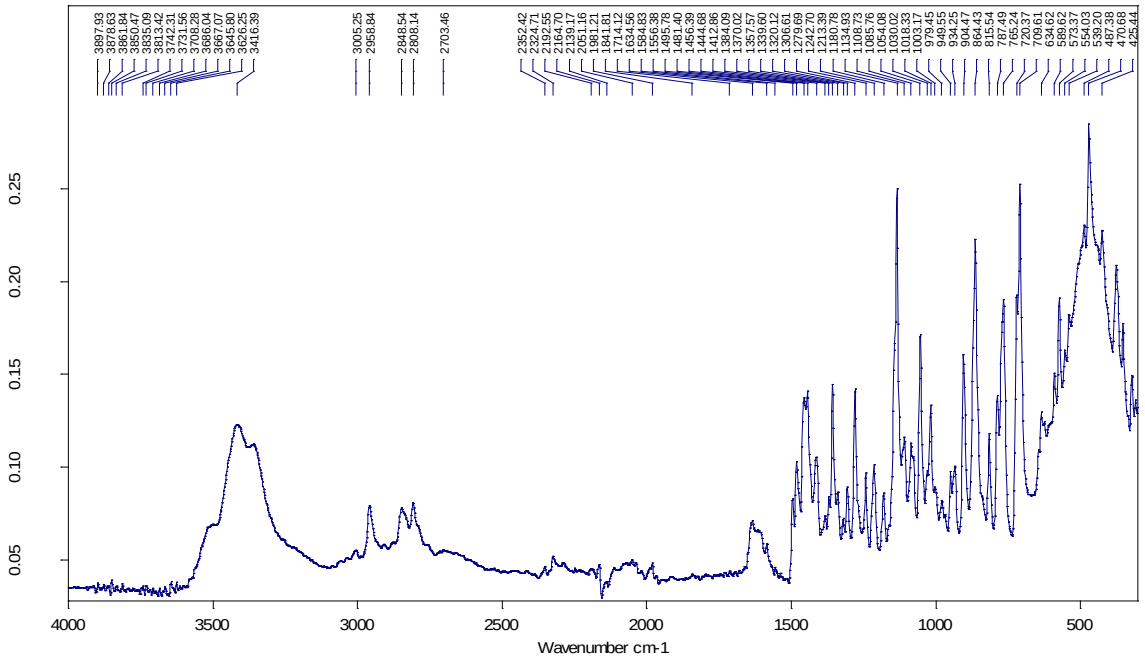
HMBC-RMN (D_2O) (δ/ppm)



Espectro de masas ESI+

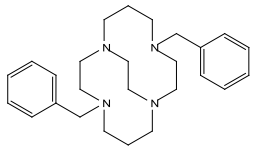


Espectro IR

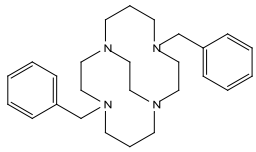


4,11-dibencil-1,4,8,11-tetraazabiciclo[6.6.2]hexadecano (**26**)

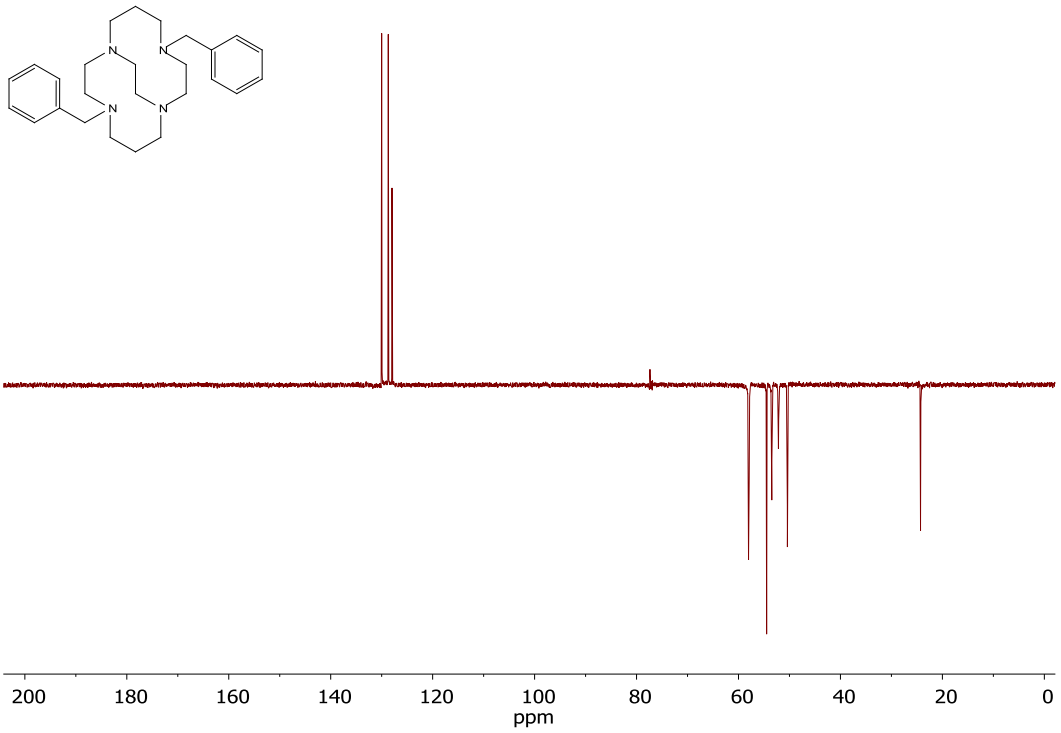
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



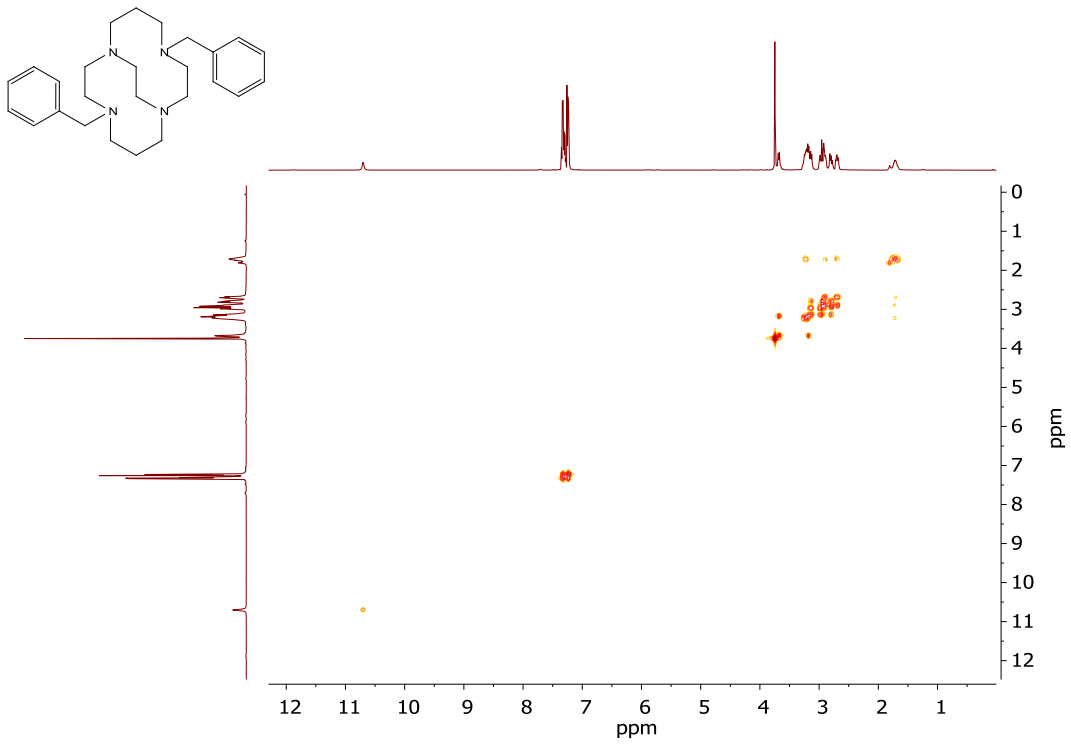
^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)



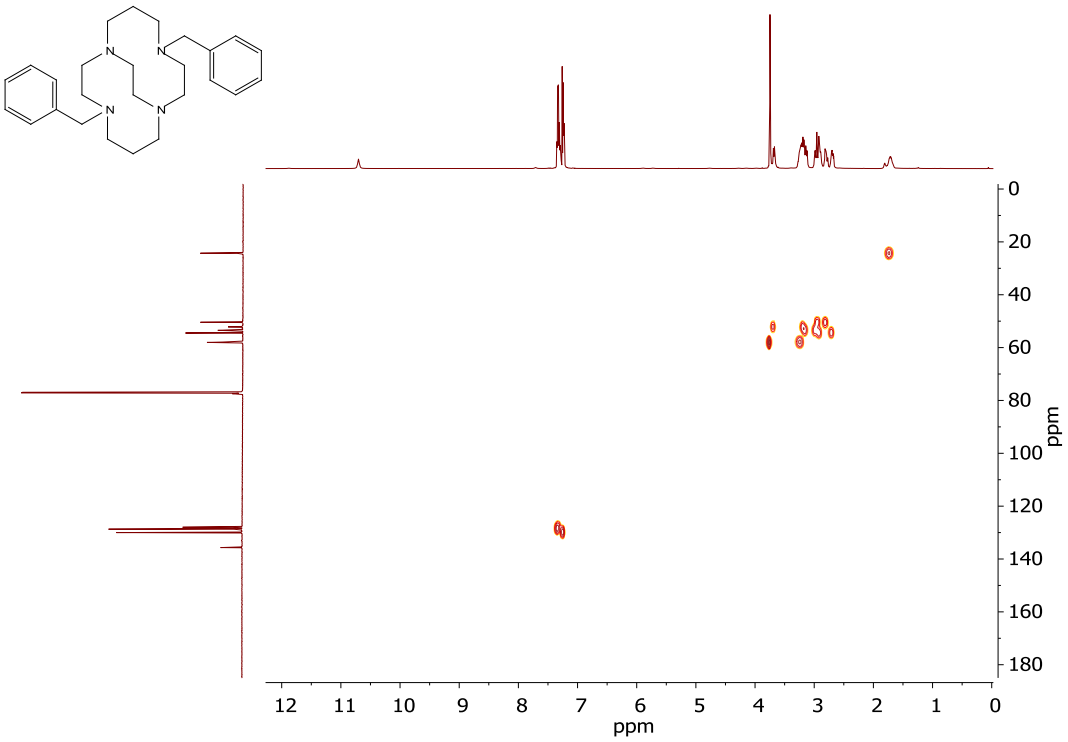
DEPT-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



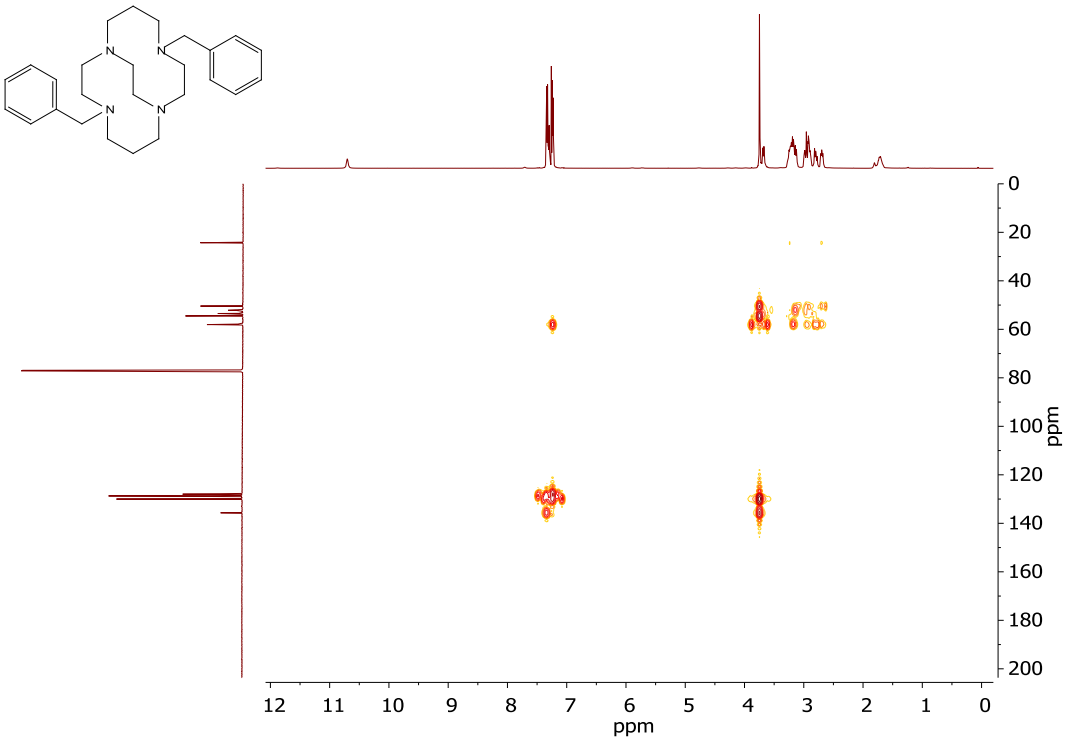
COSY-RMN ($CDCl_3$) (δ/ppm)



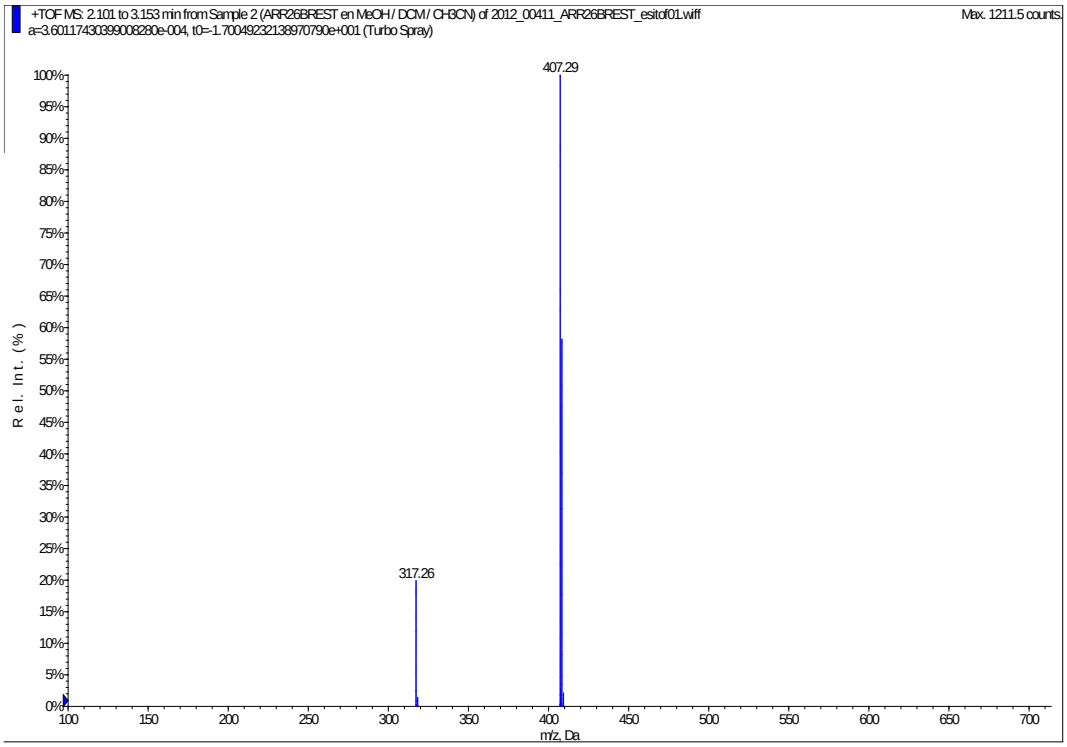
HSQC-RMN ($CDCl_3$) (δ/ppm)



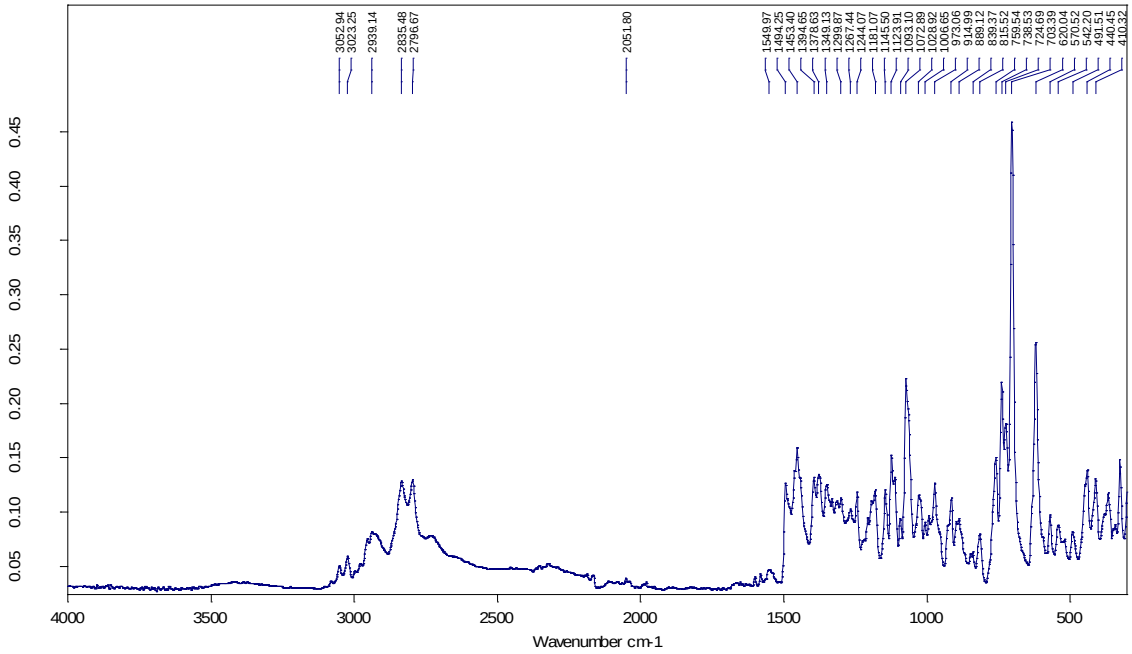
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

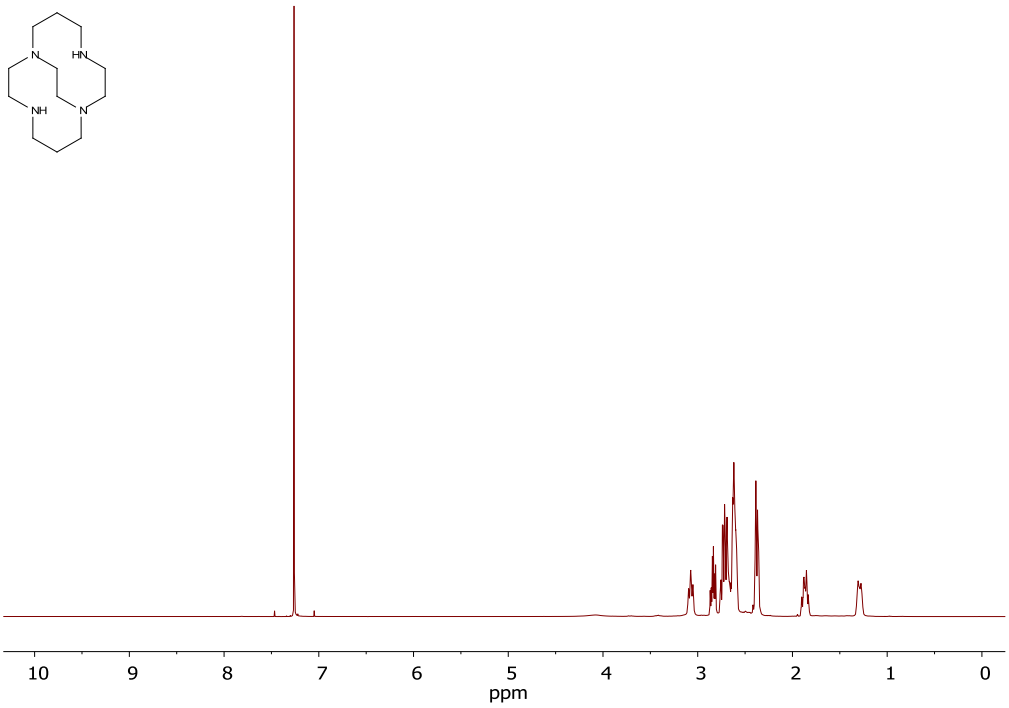


Espectro IR

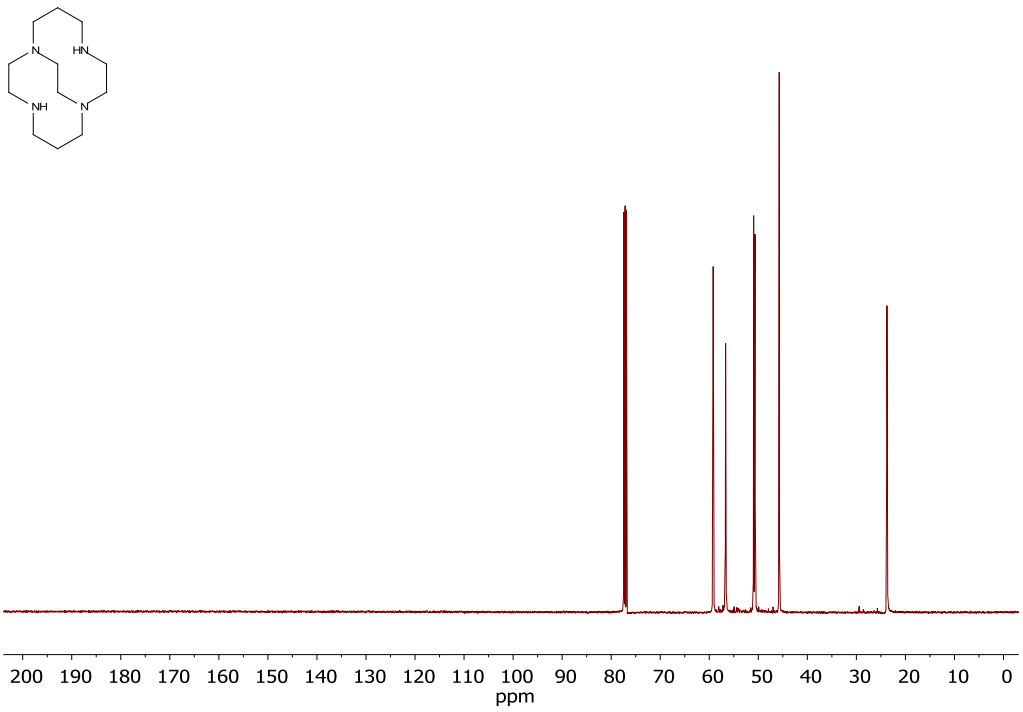


1,4,8,11-tetraazabiciclo[6.6.2]hexadecano – ciclam cross-bridged – (**27**)

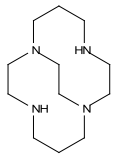
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)

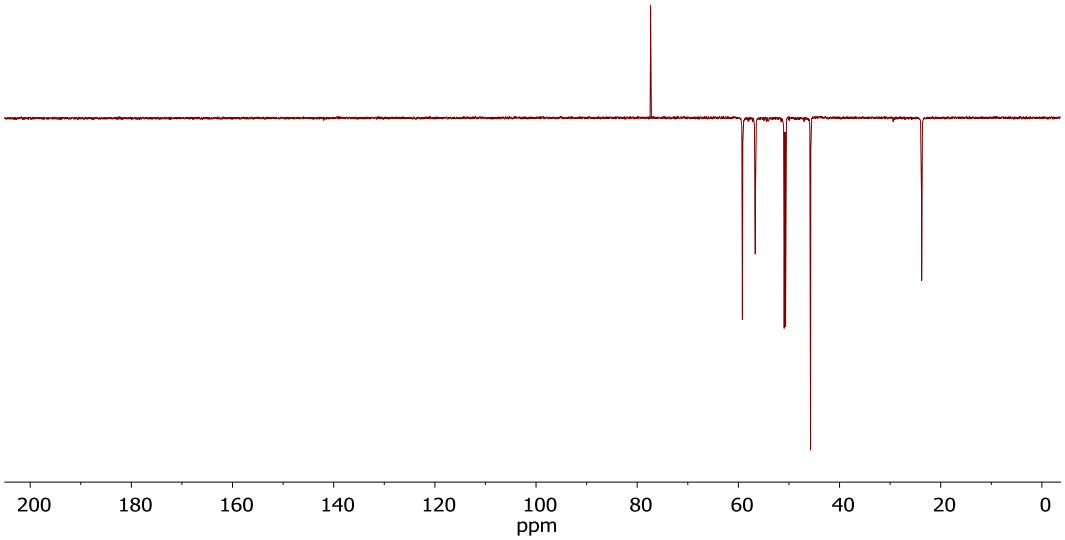


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

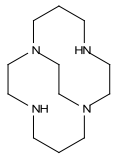


DEPT-RMN ($CDCl_3$) (δ/ppm)

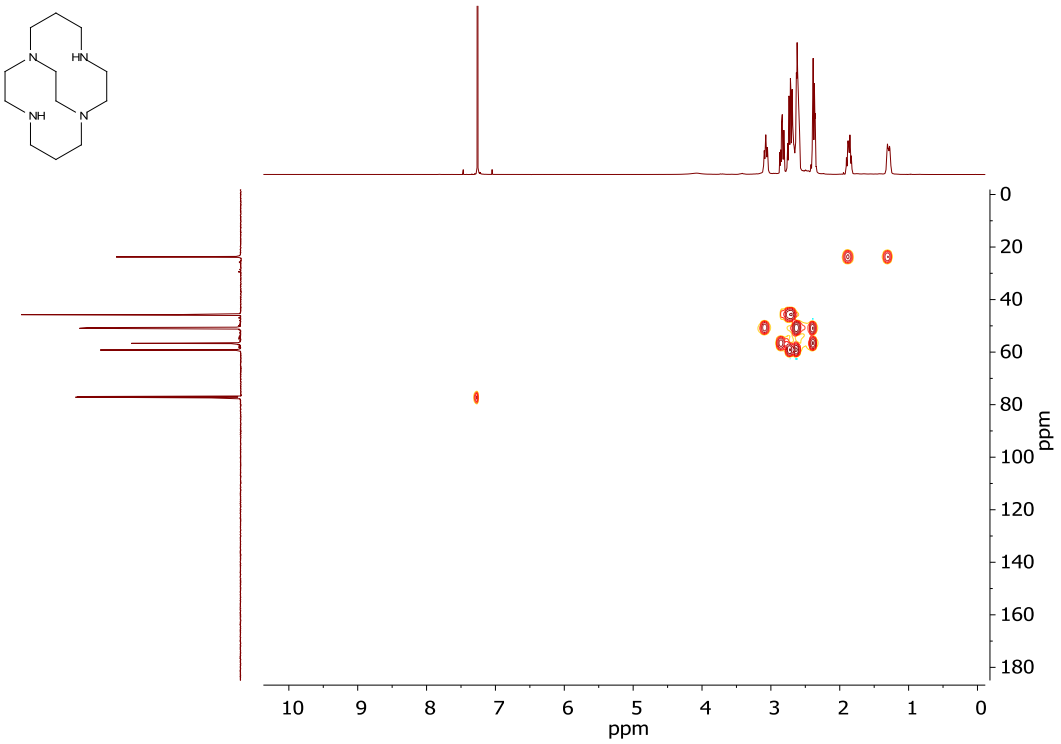




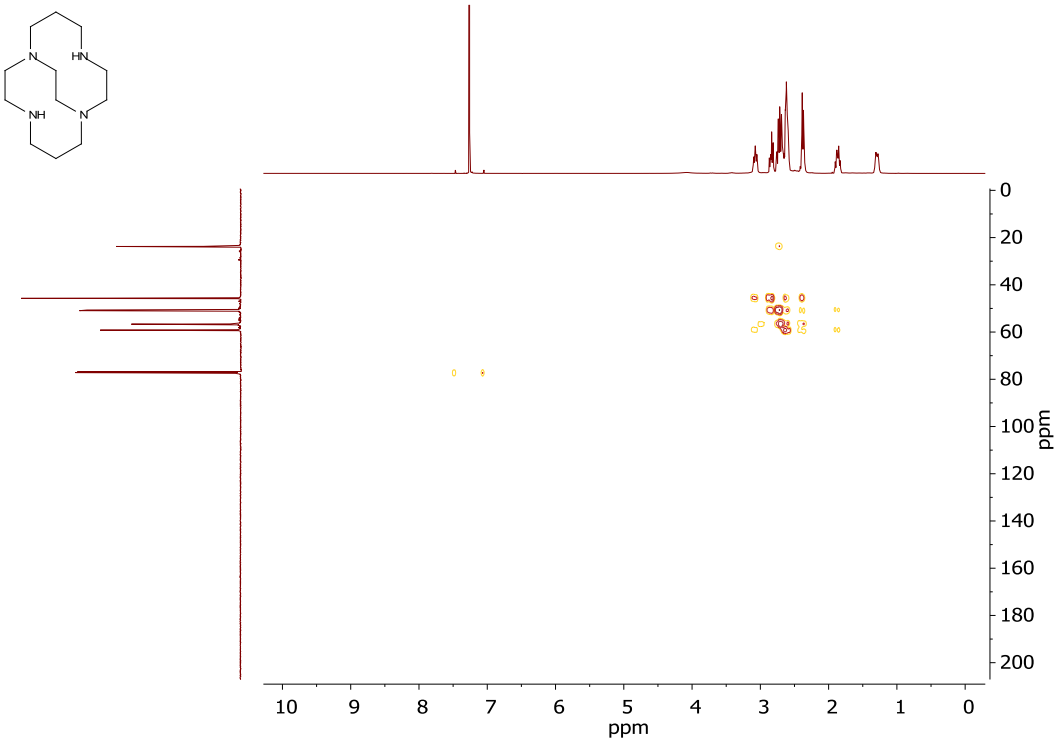
COSY-RMN ($CDCl_3$) (δ/ppm)



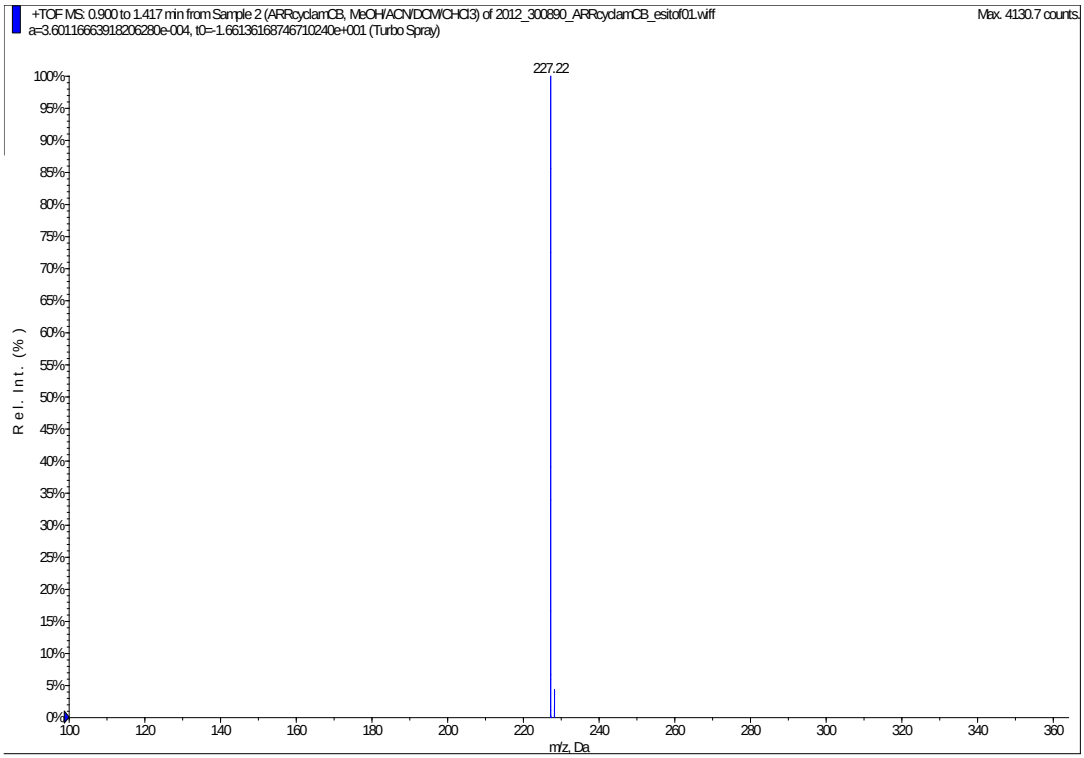
HSQC-RMN ($CDCl_3$) (δ/ppm)



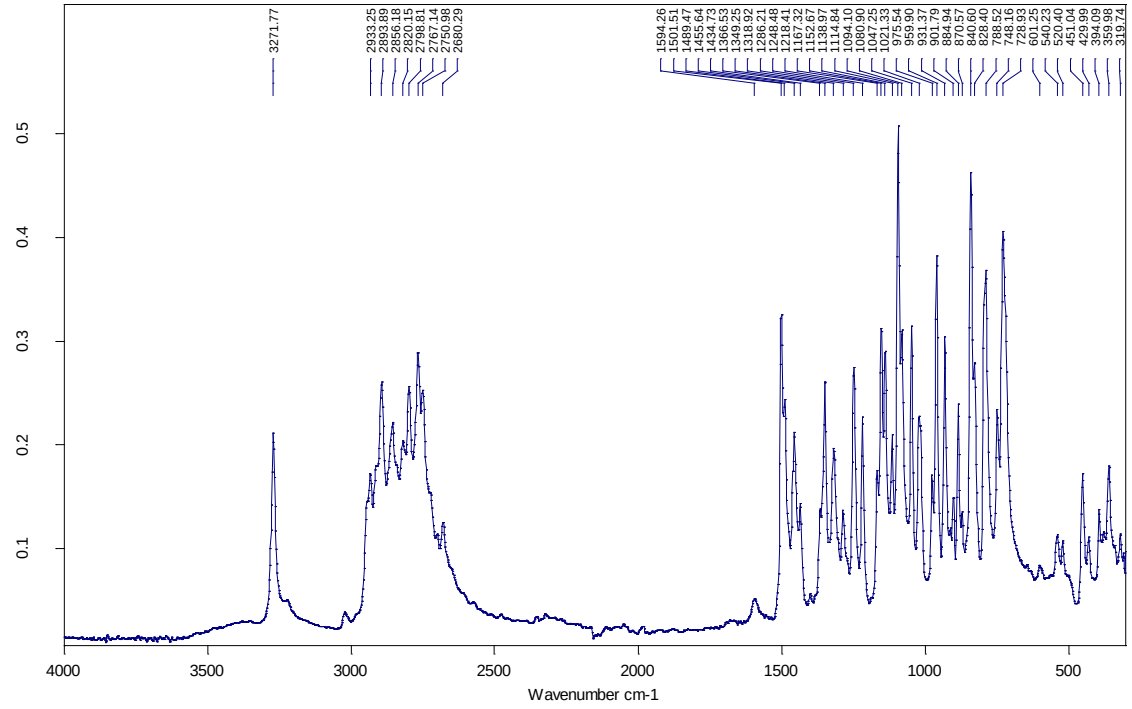
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

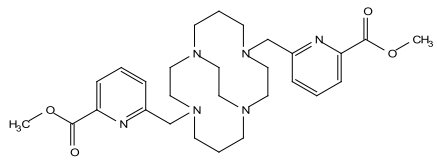


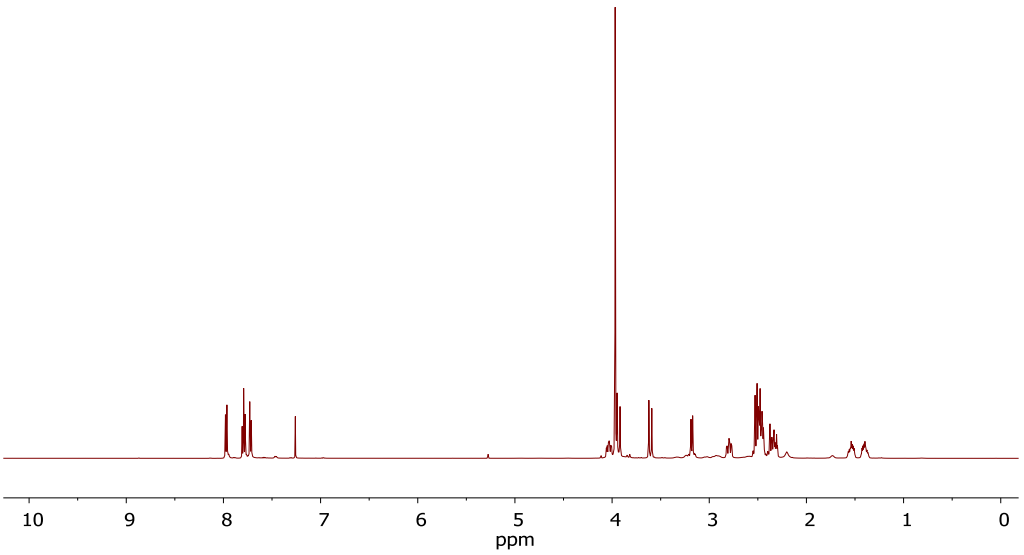
Espectro IR



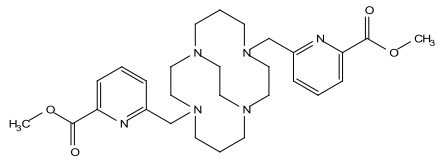
Dimetil 6,6'-((1,4,8,11-tetraazabiciclo[6.6.2]hexadecano-4,11-diil)bis(metilen))dipicolinato (**28**)

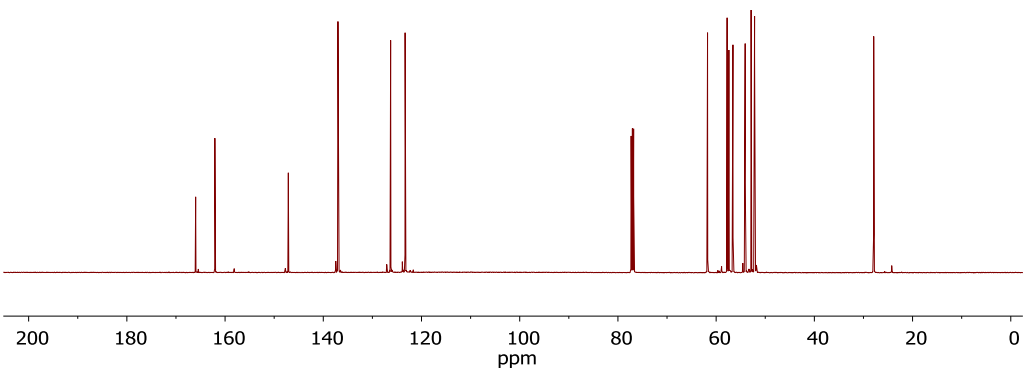
^{1}H-RMN ($CDCl_3$, 500 MHz) (δ/ppm)



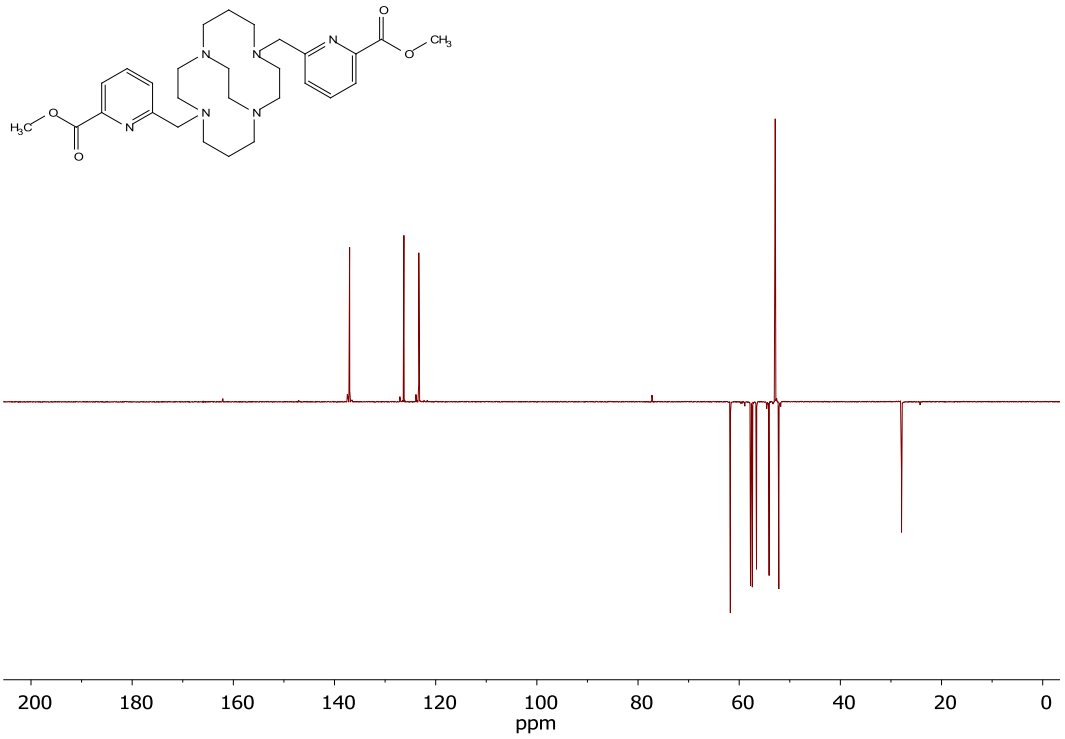


^{13}C-RMN ($CDCl_3$, 125,8 MHz) (δ/ppm)

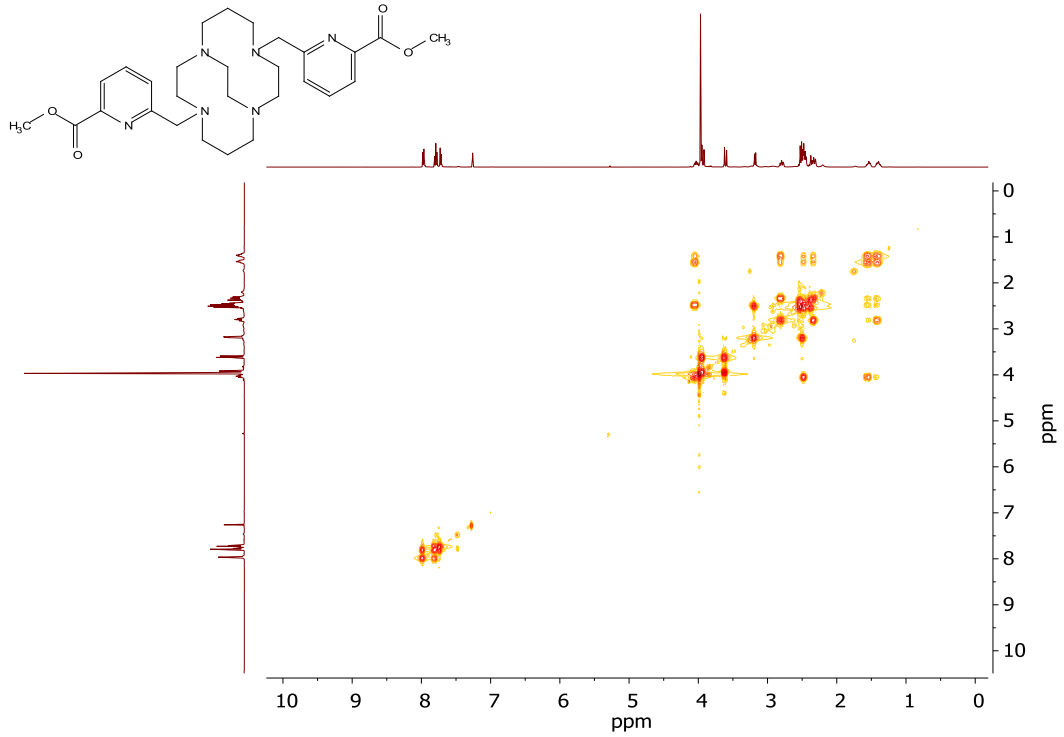




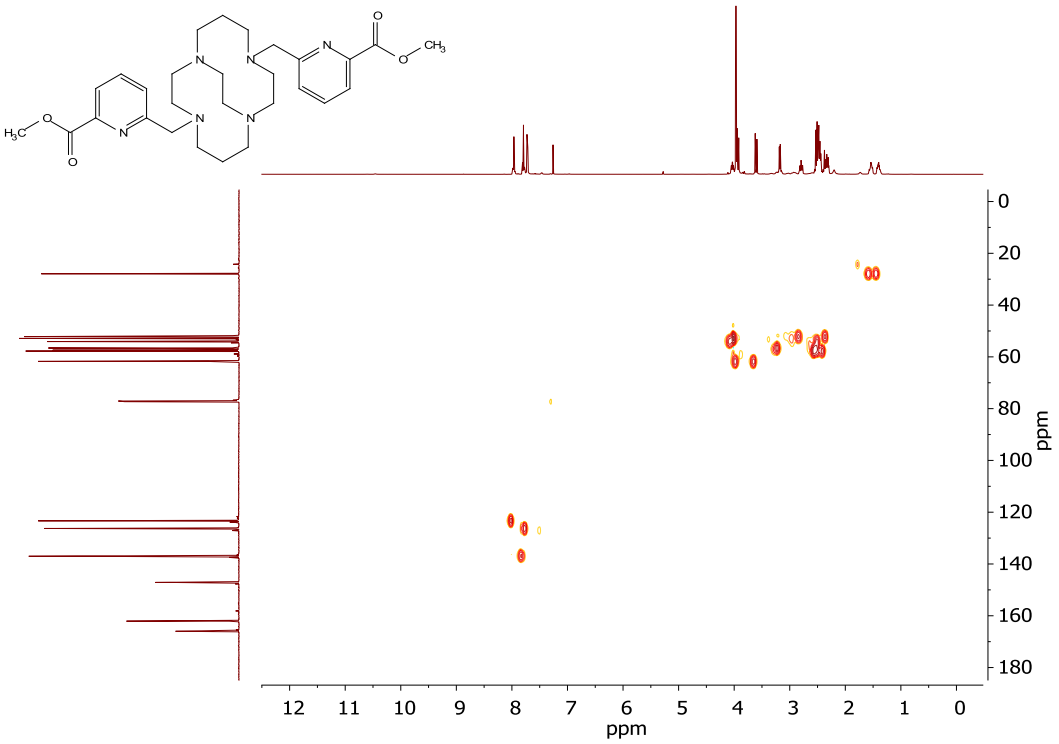
DEPT-RMN ($CDCl_3$) (δ/ppm)



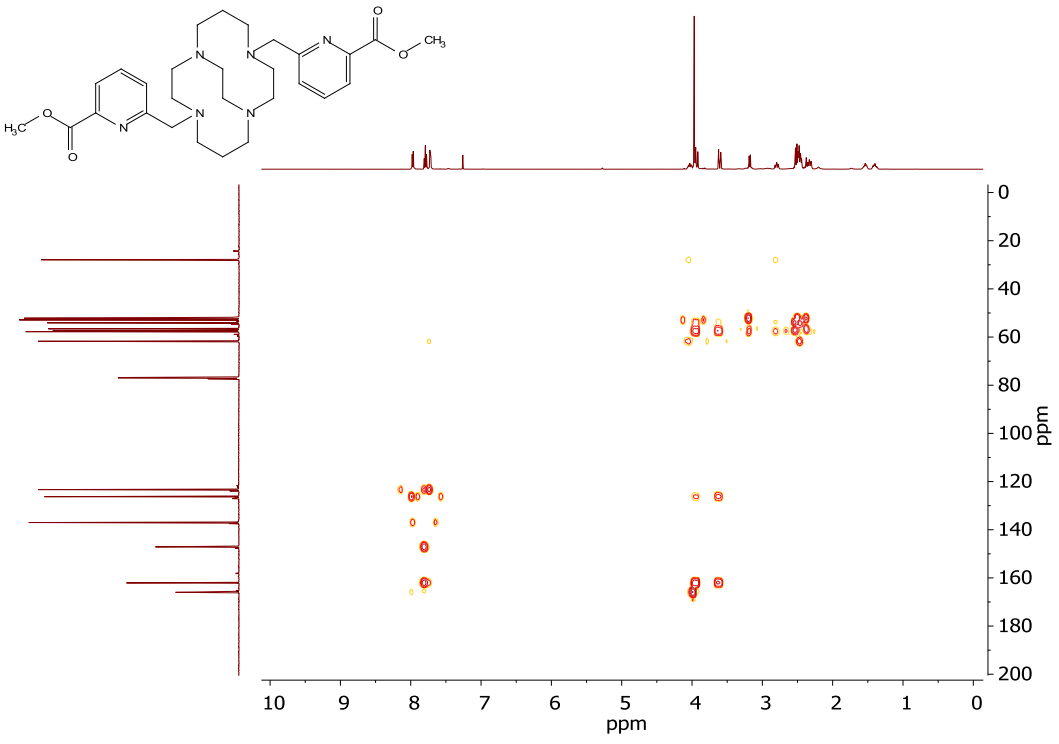
COSY-RMN ($CDCl_3$) (δ/ppm)



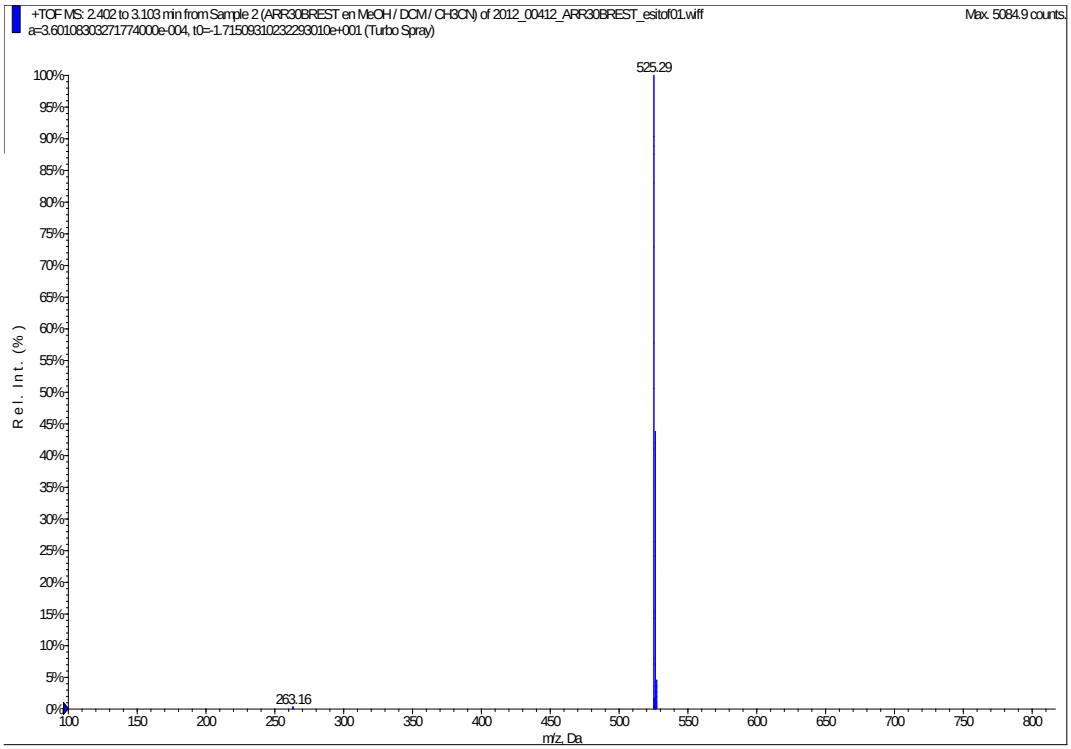
HSQC-RMN ($CDCl_3$) (δ/ppm)



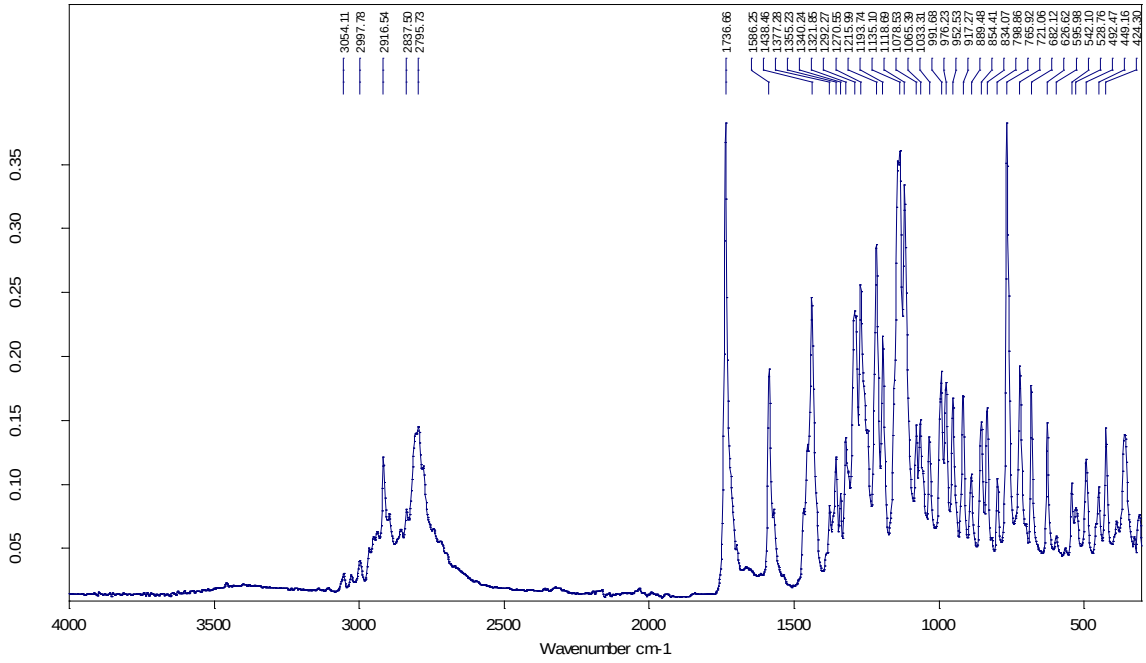
HMBC-RMN ($CDCl_3$) (δ/ppm)



Espectro de masas ESI+

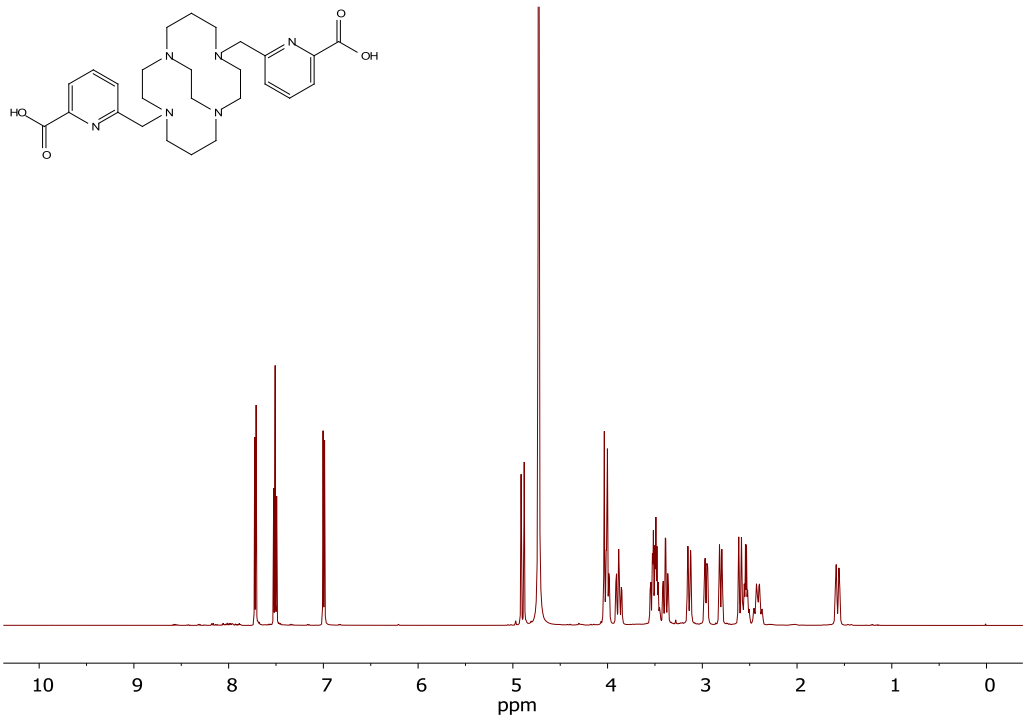


Espectro IR

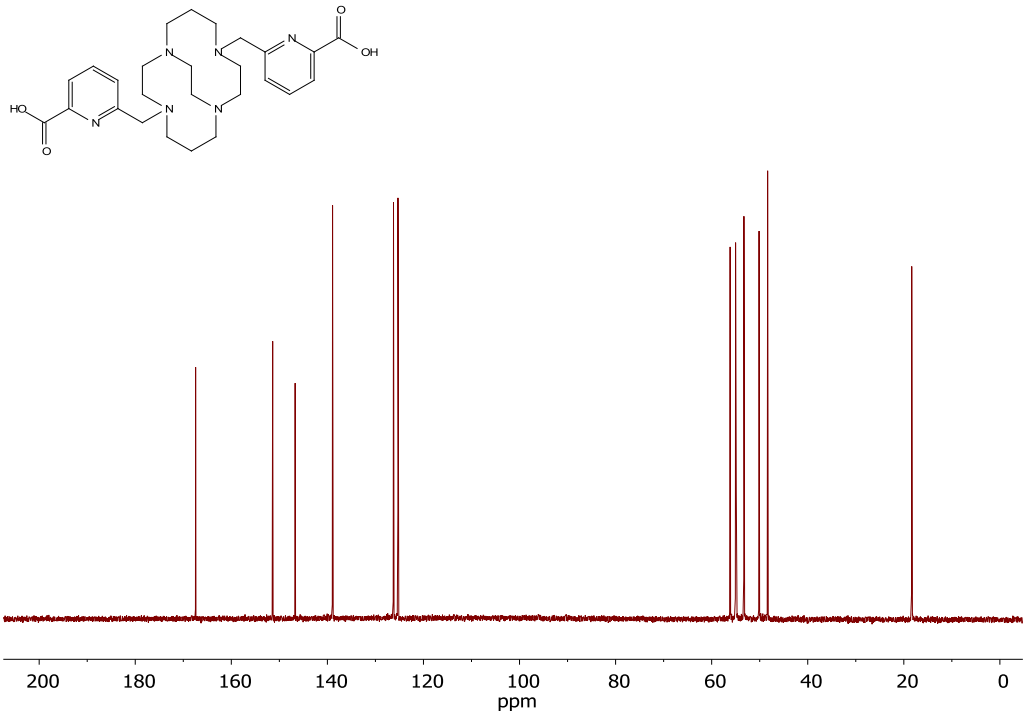


Ácido 6,6'-((1,4,8,11-tetraazabiciclo[6.6.2]hexadecano-4,11-diil)bis(metilen))dipicolínico (H_2cb-tedpa·5HCl·H_2O)

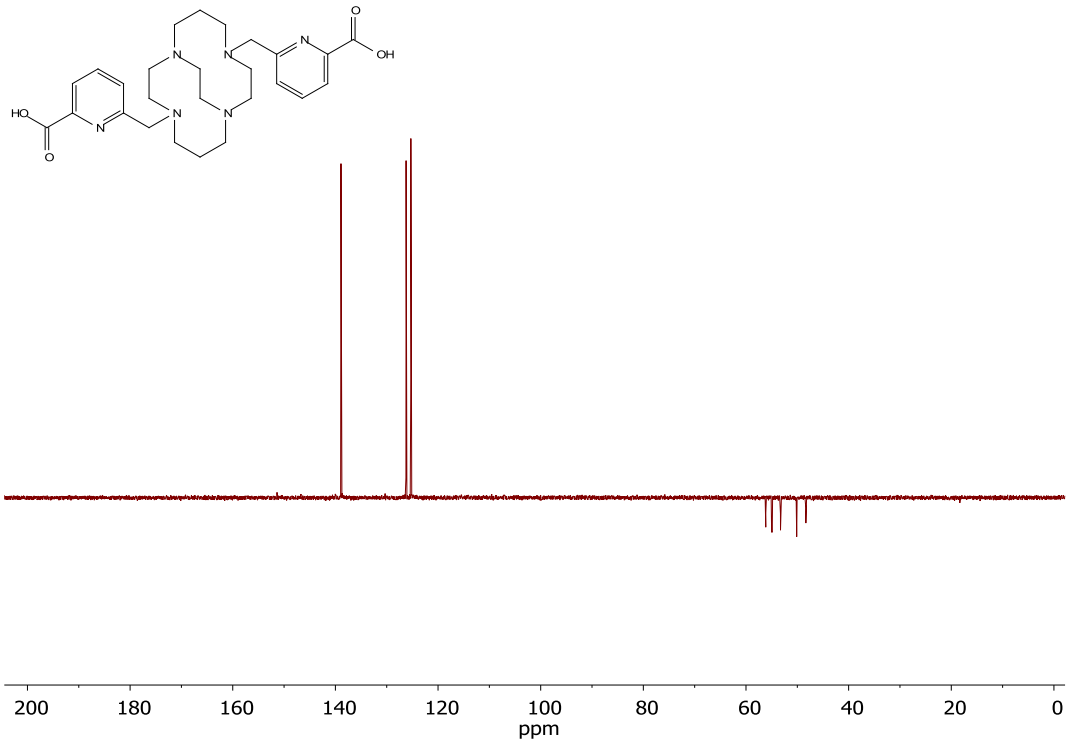
^{1}H-RMN (D_2O, 500 MHz, pD = 0,9) (δ/ppm)



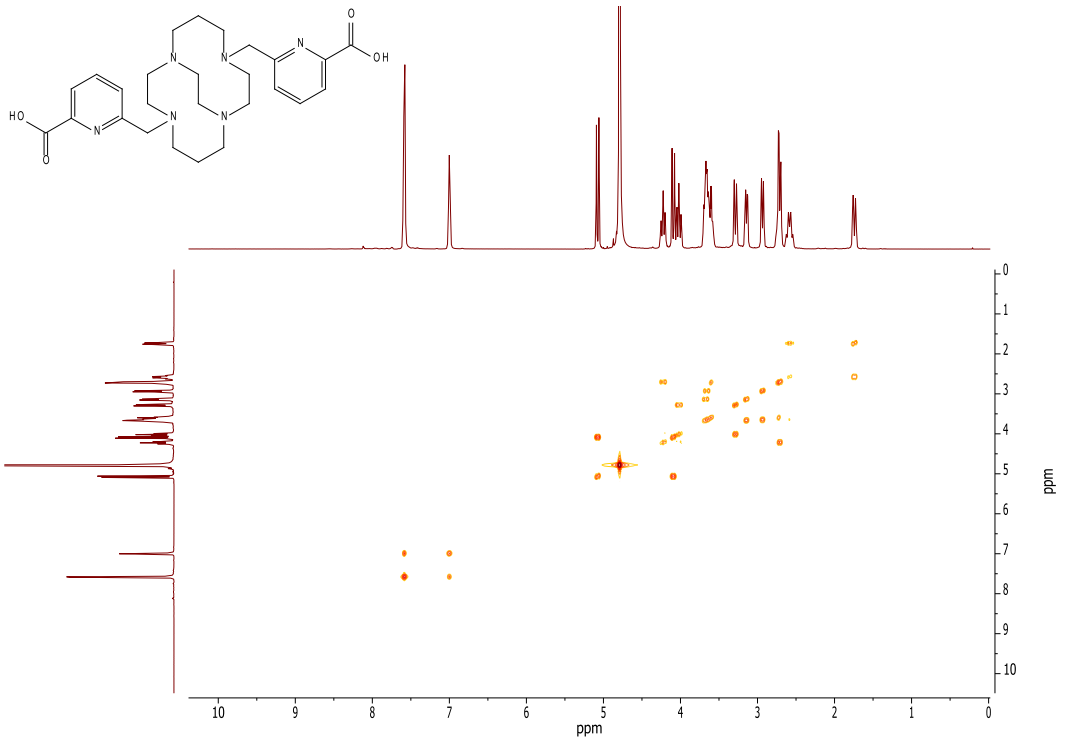
^{13}C-RMN (D_2O, 125,8 MHz, pD = 0,9) (δ/ppm)



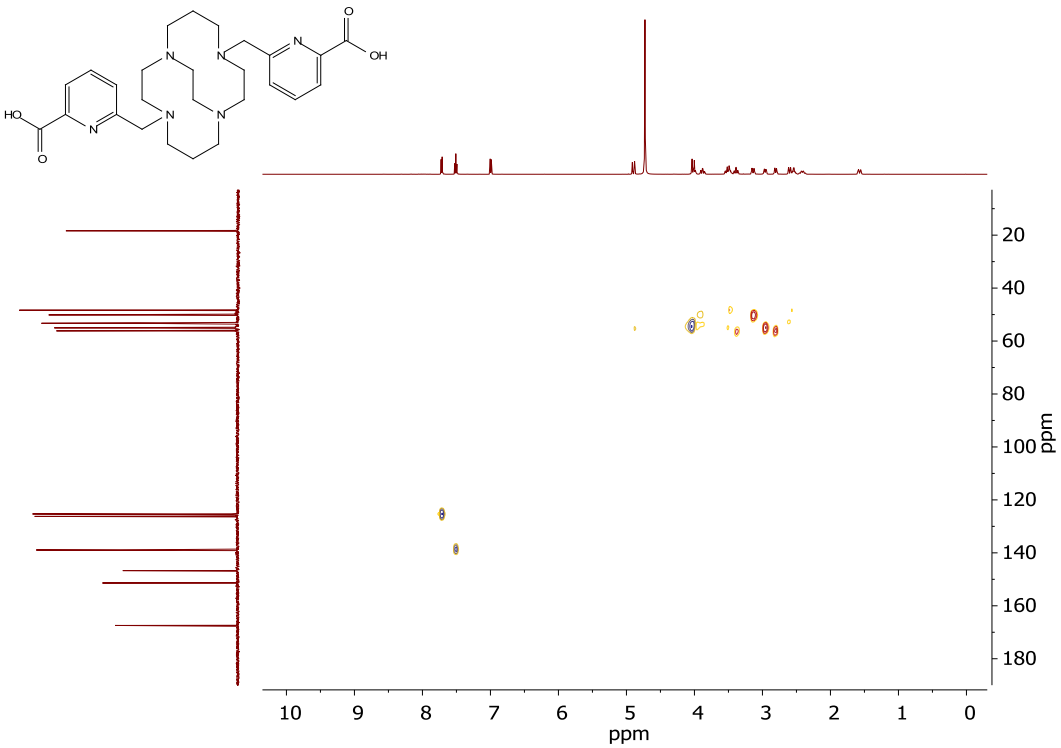
DEPT-RMN (D_2O, pD = 0,9) (δ/ppm)



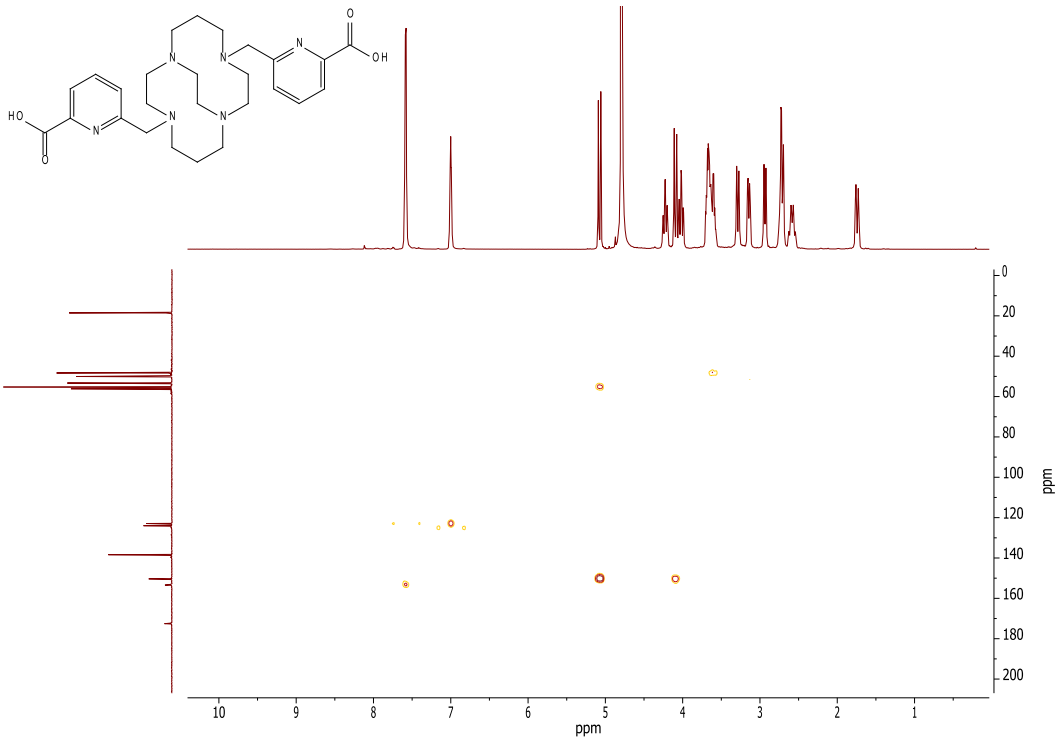
COSY-RMN (D_2O, pD = 0,9) (δ/ppm)



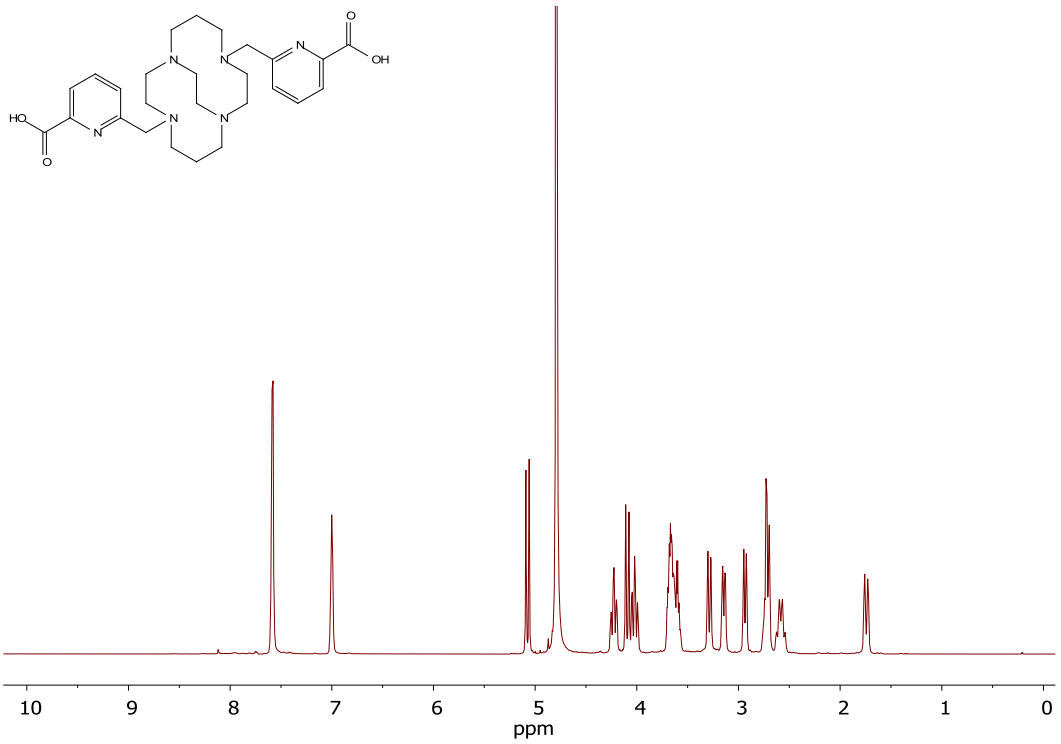
HSQC-RMN (D_2O, pD = 0,9) (δ/ppm)



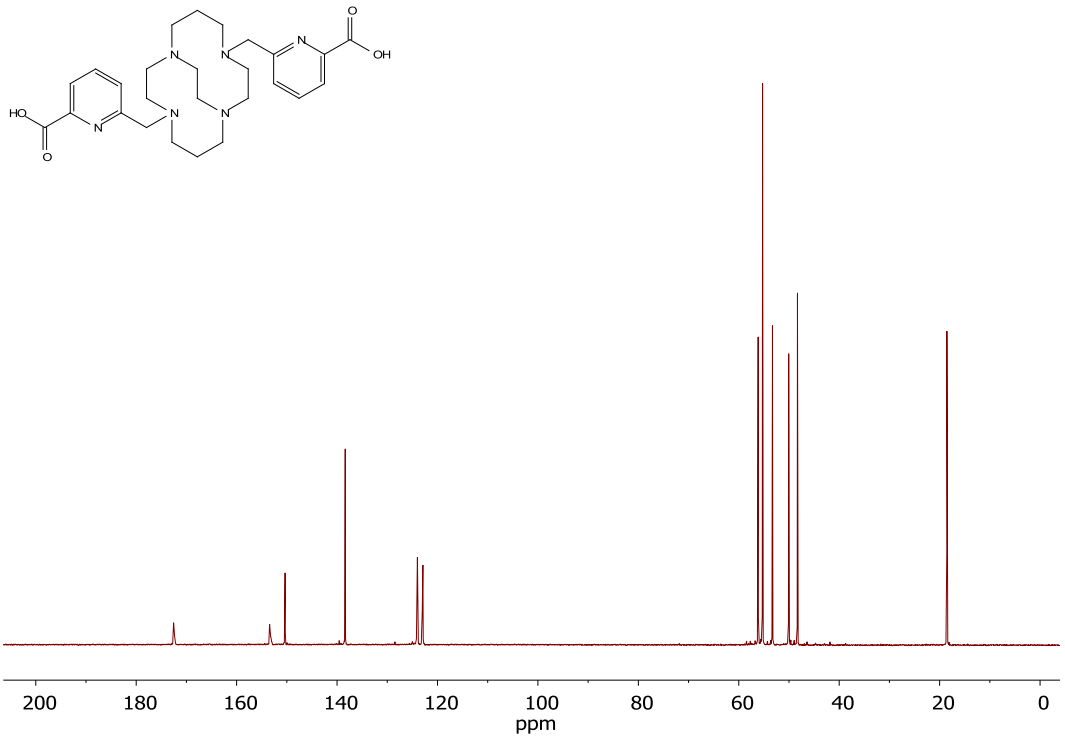
HMBC-RMN (D_2O, pD = 0,9) (δ/ppm)



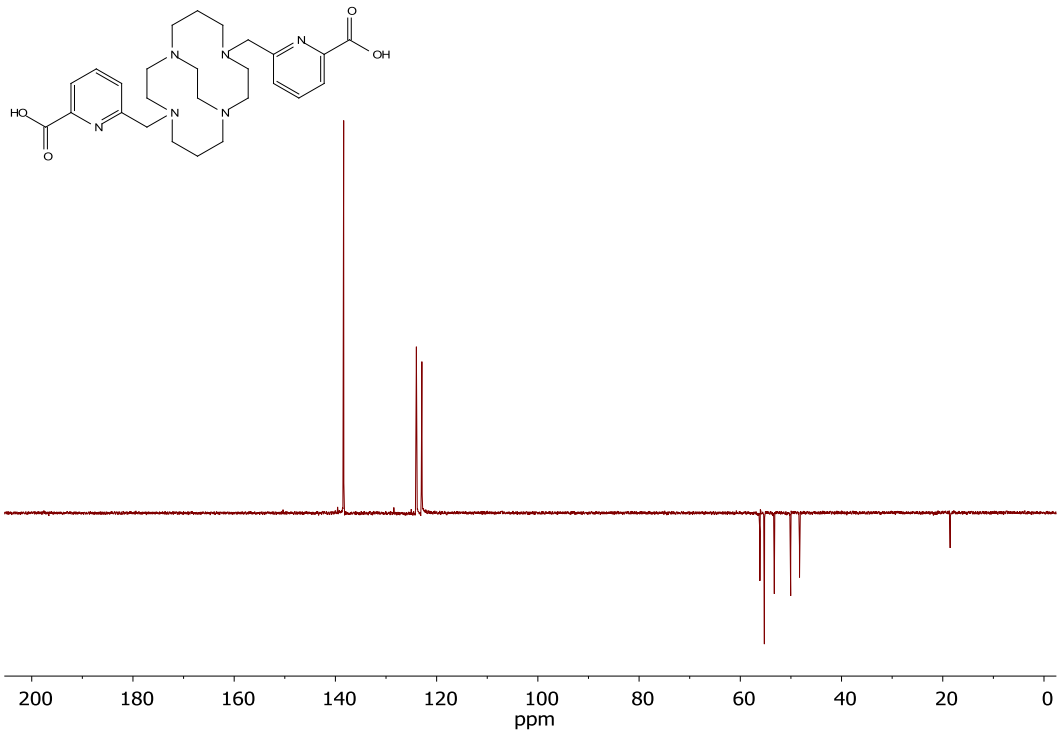
^{1}H-RMN (D_2O, 500 MHz, pD = 7,0) (δ/ppm)



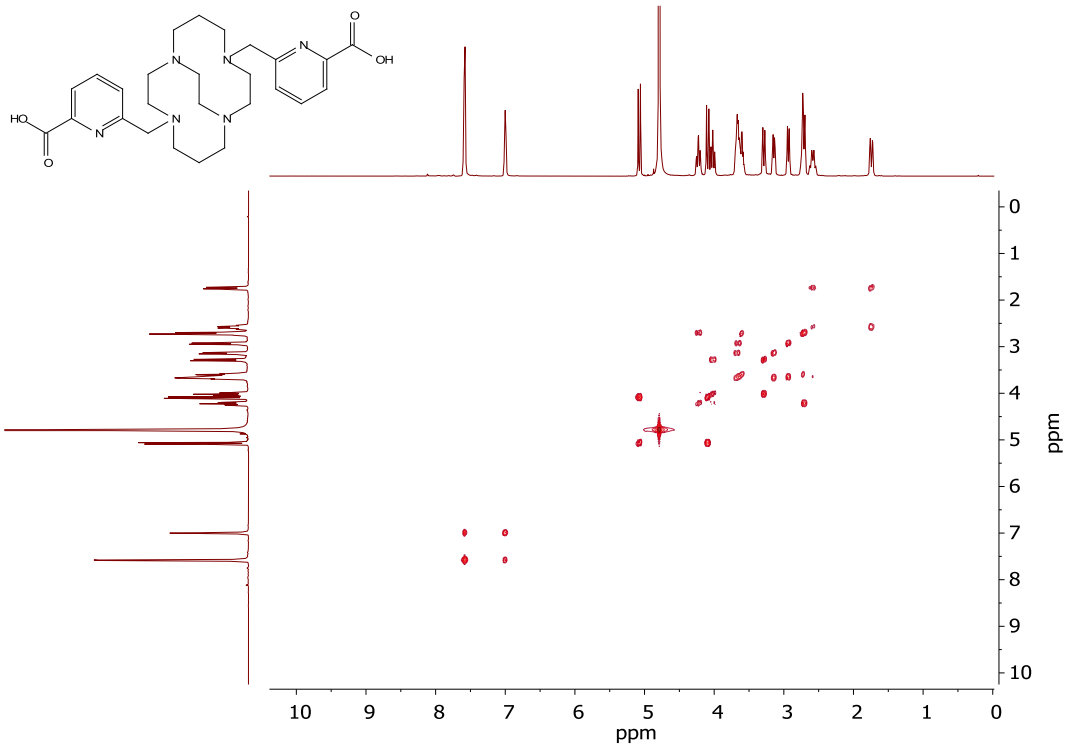
^{13}C-RMN (D_2O, 125,8 MHz, pD = 7,0) (δ/ppm)



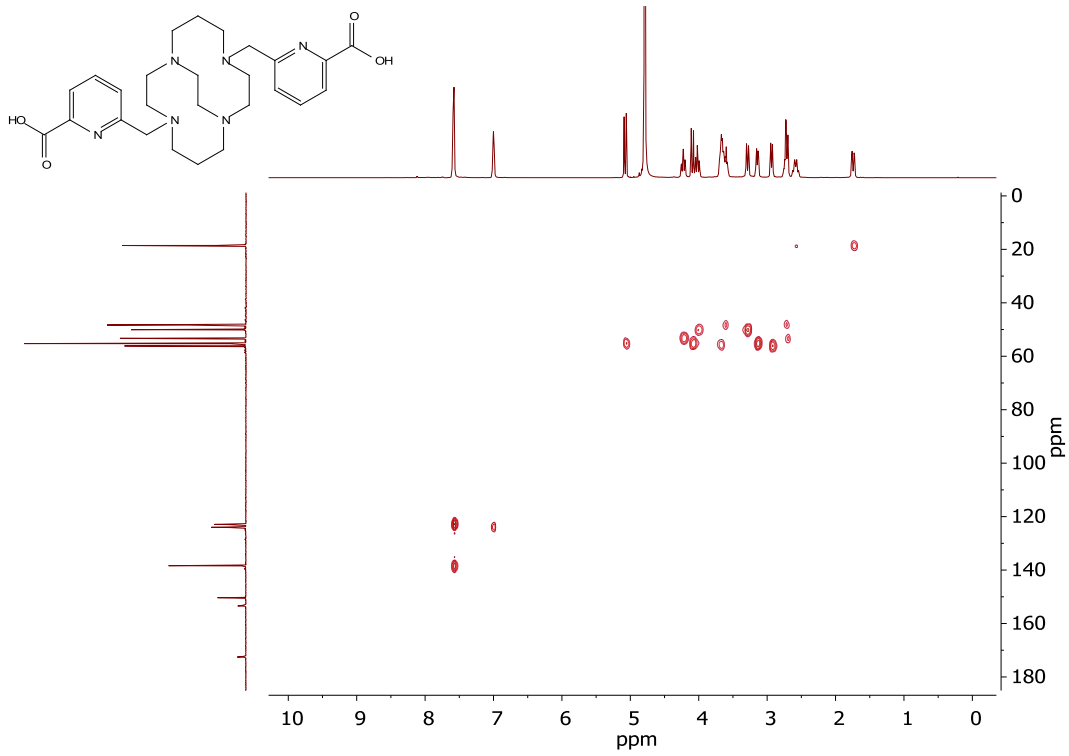
DEPT-RMN (D_2O, pD = 7,0) (δ/ppm)



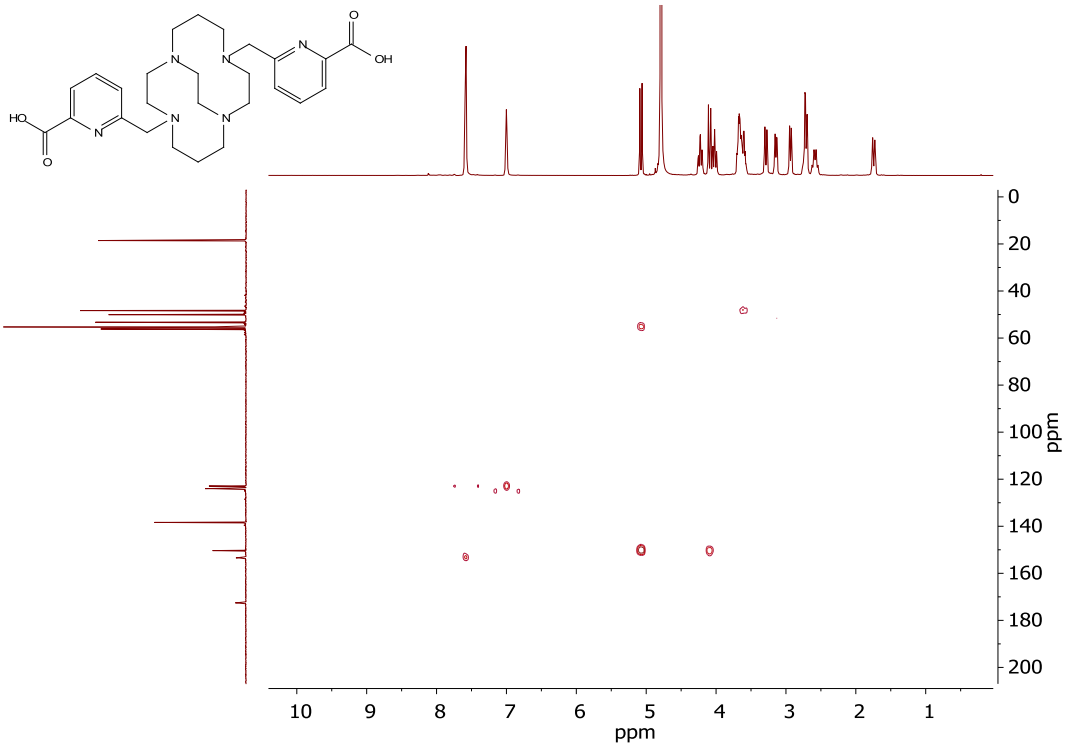
COSY-RMN (D_2O, pD = 7,0) (δ/ppm)



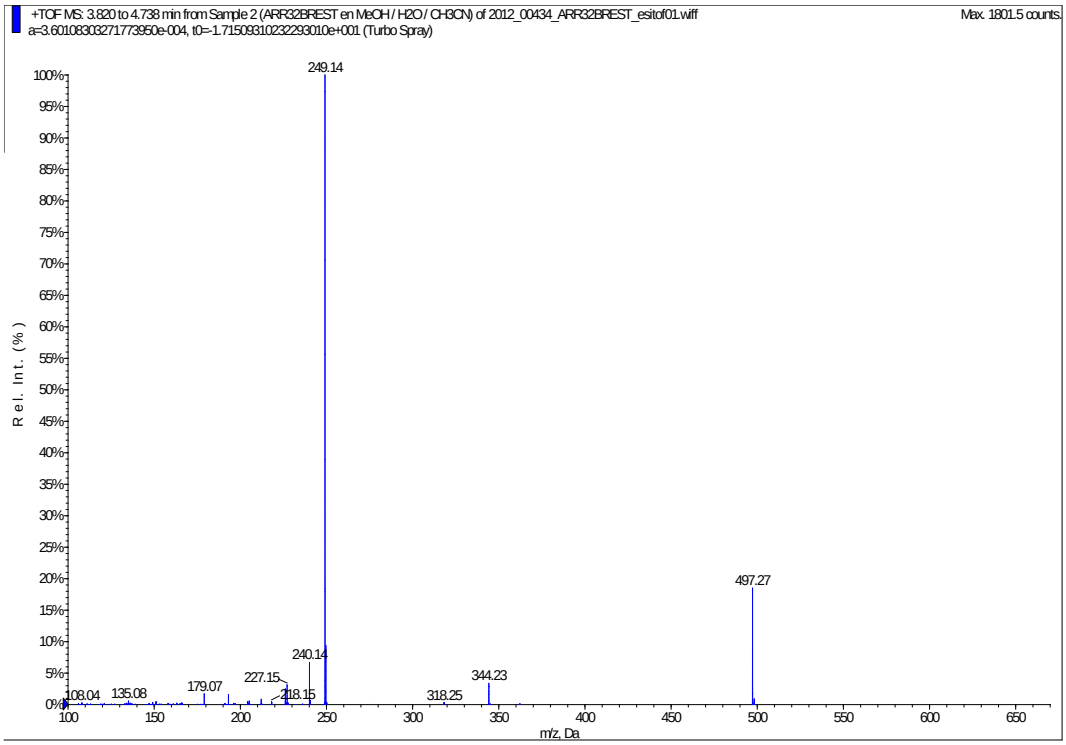
HSQC-RMN (D_2O, pD = 7,0) (δ/ppm)



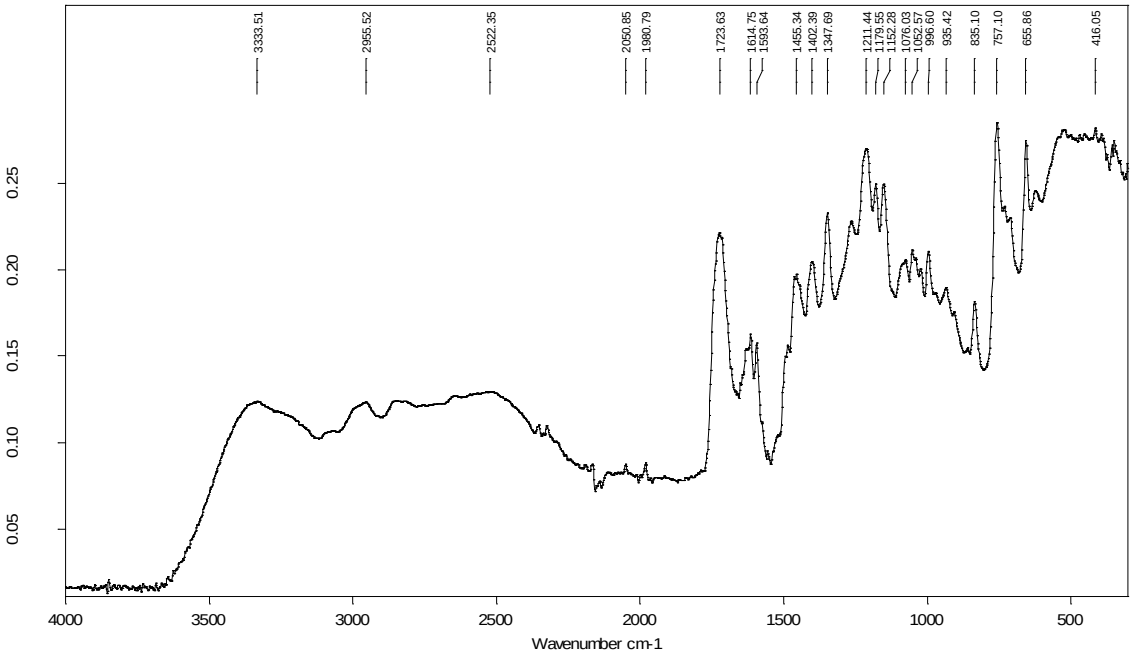
HMBC-RMN (D_2O, pD = 7,0) (δ/ppm)



Espectro de masas ESI+

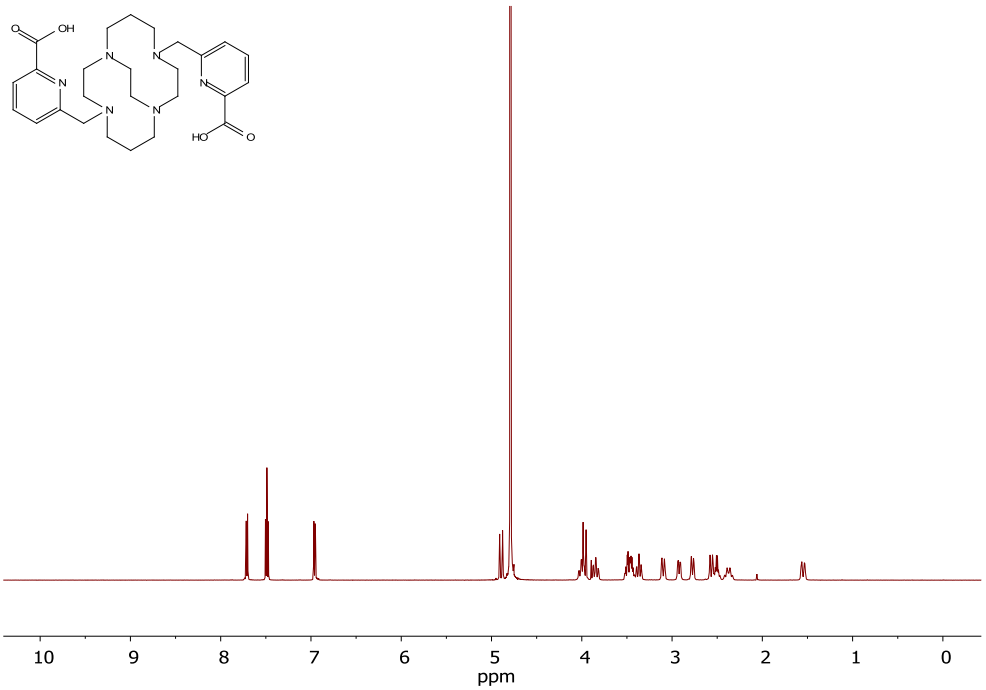


Espectro IR

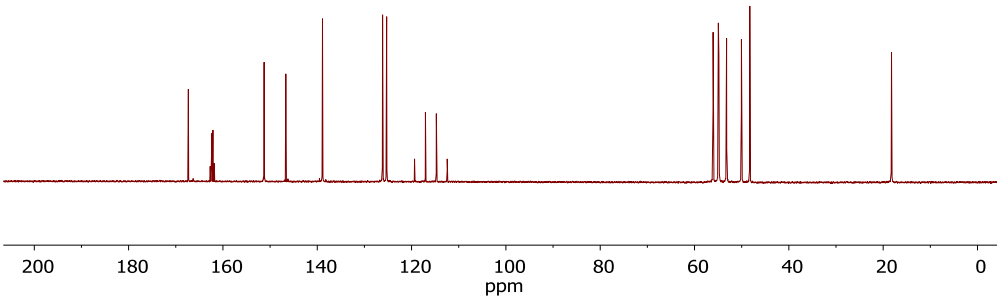


Ácido 6,6'-((1,4,8,11-tetraazabiciclo[6.6.2]hexadecano-4,11-diil)bis(metilen))dipicolínico (H_2cb-tedpa·6TFA·H_2O)

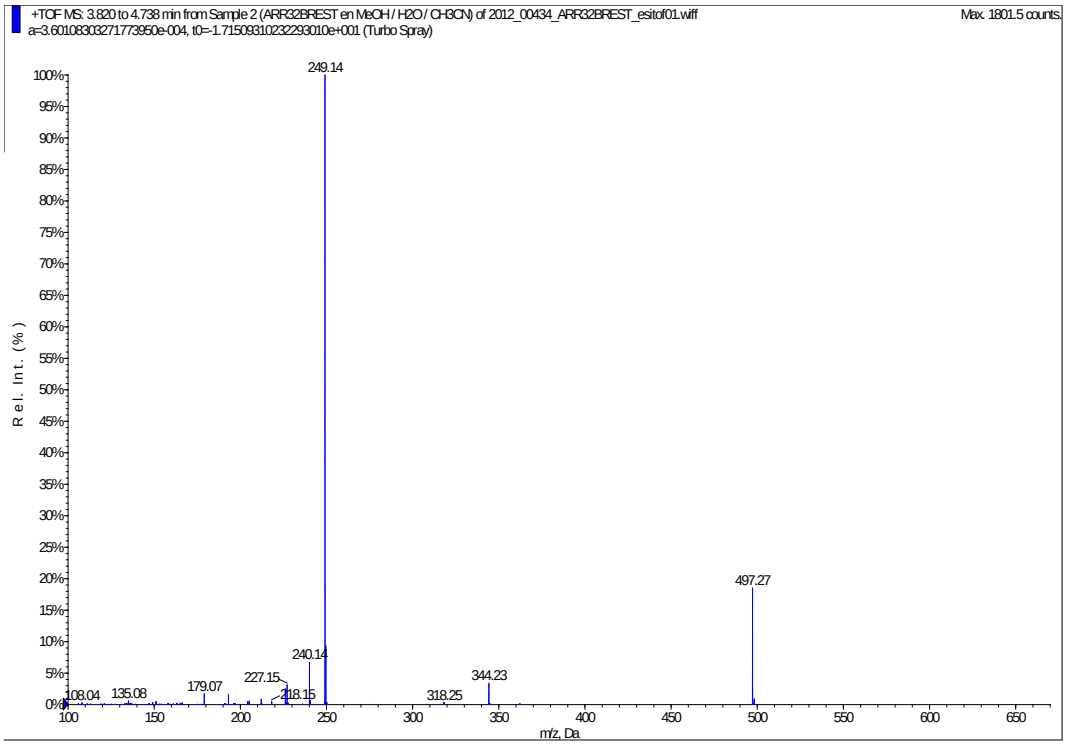
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



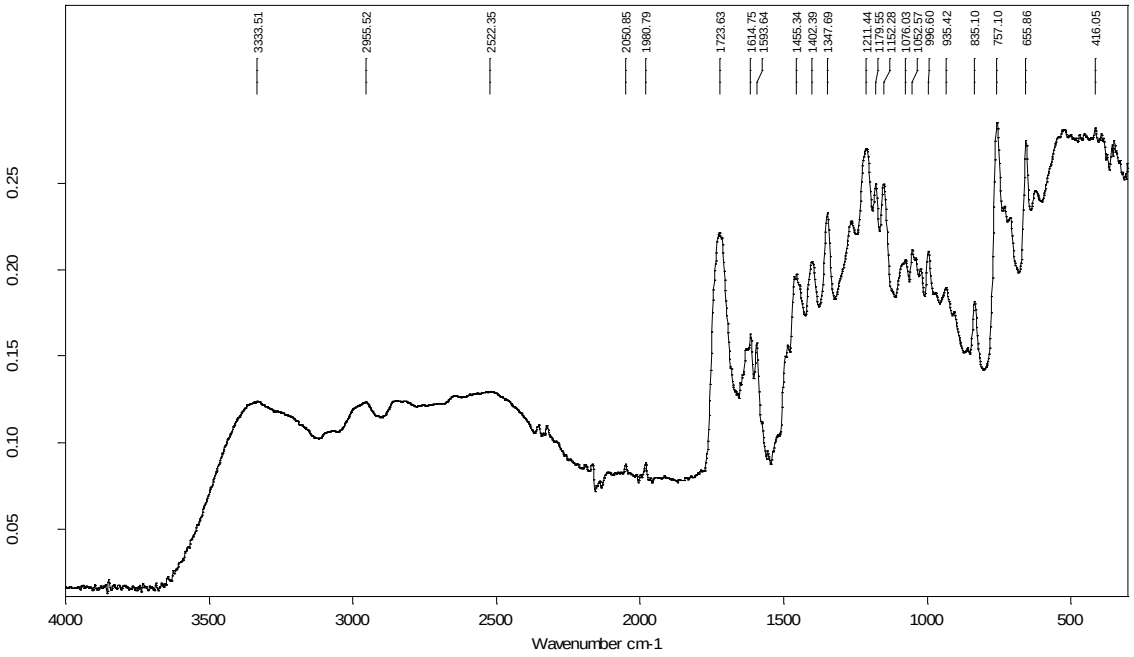
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



Espectro de masas ESI+



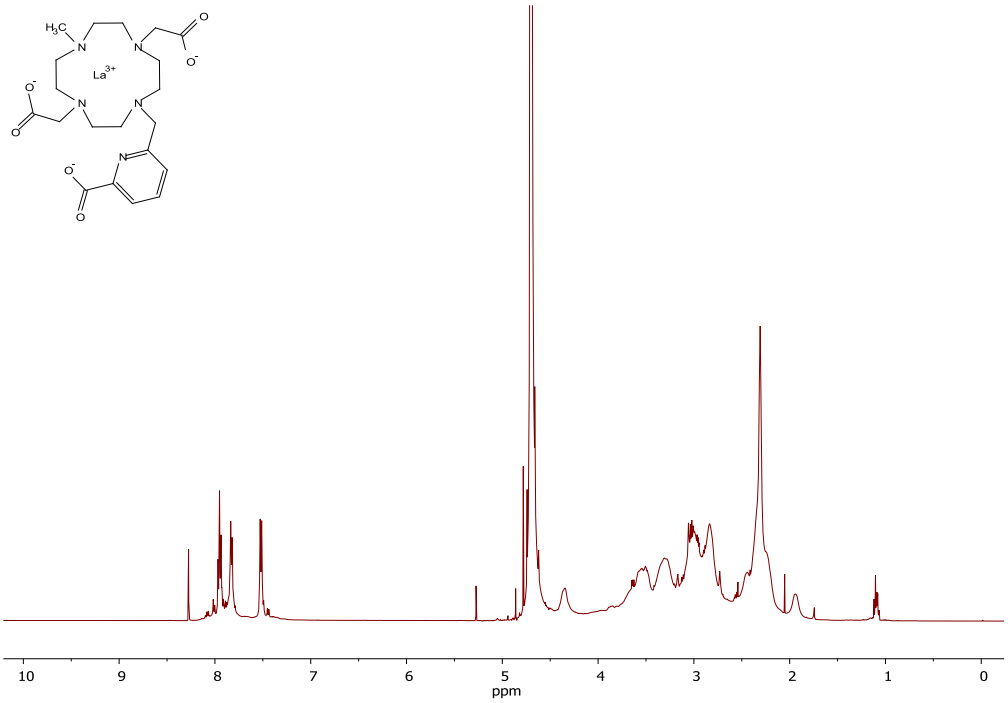
Espectro IR



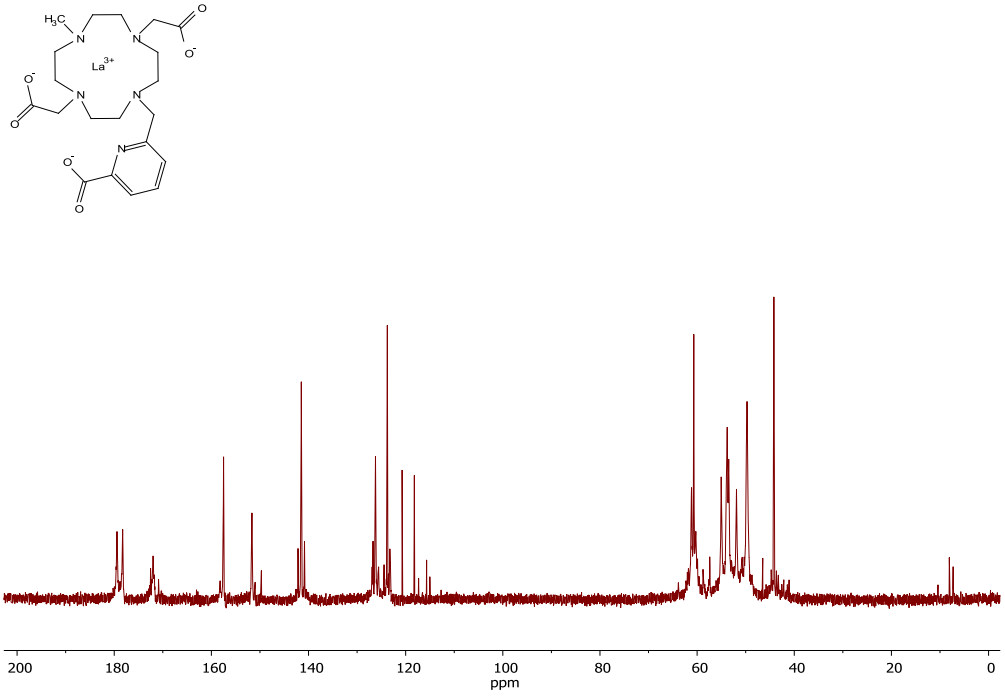
Espectros de RMN, Masas e Infrarrojo de los Complejos

[La(1,7-Medo2ampa)]

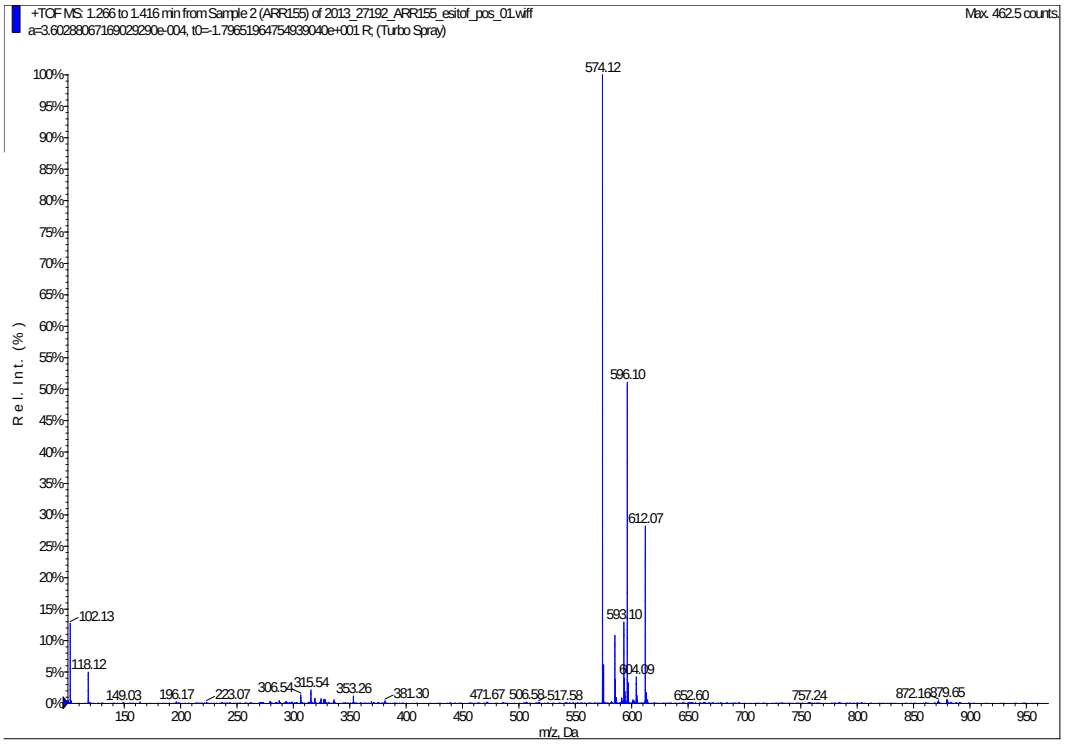
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



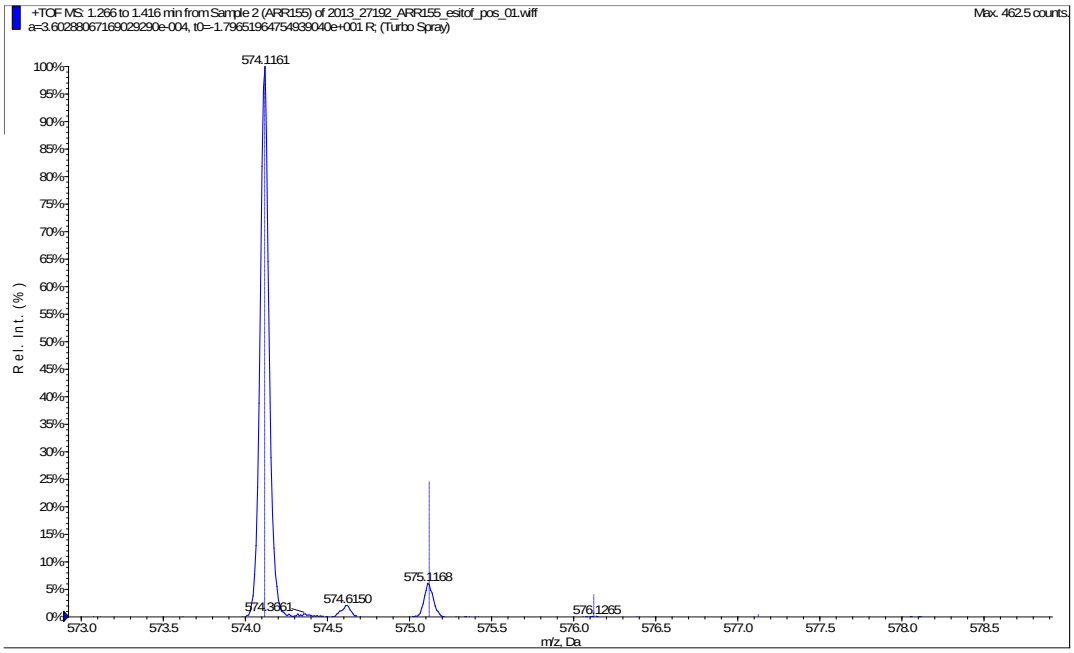
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



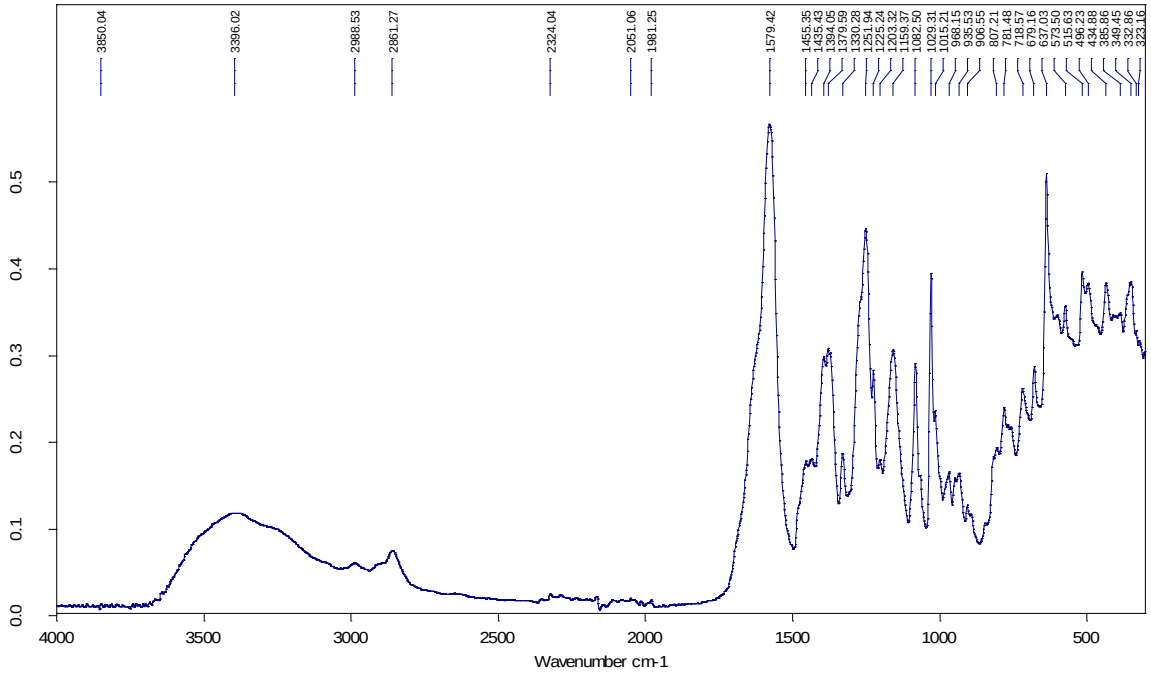
Espectro de masas ESI+



Espectro ESI+ HR

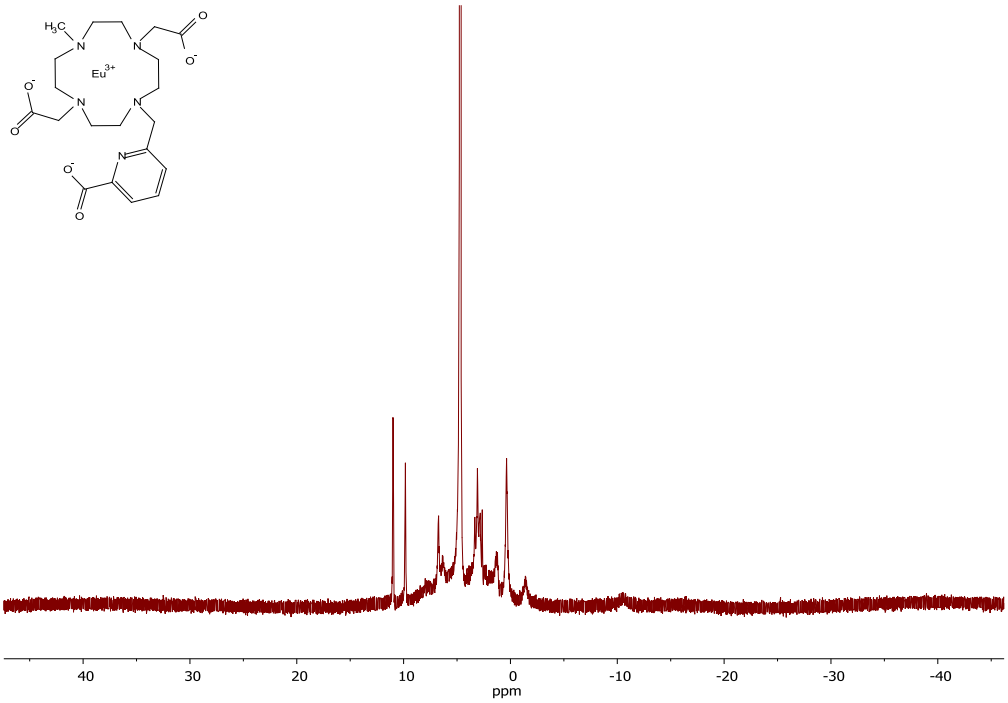


Espectro IR

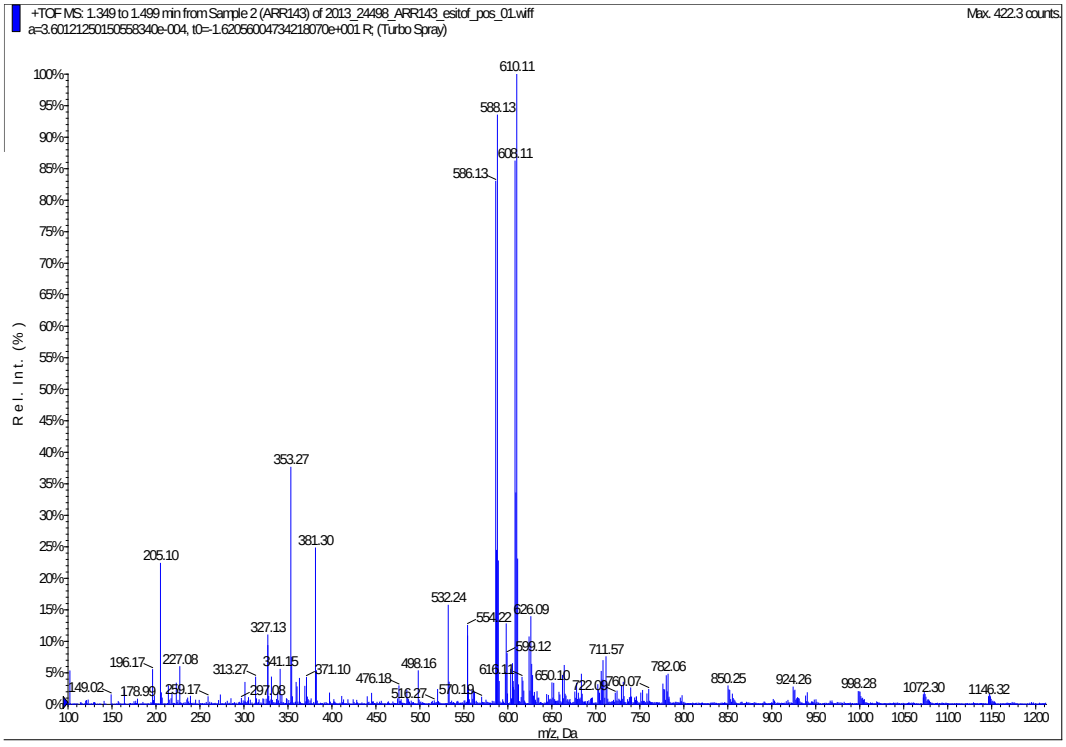

3850.04
3396.02
2988.53
2861.27
2324.04
2051.06
1981.25
1579.42
1455.35
1435.43
1394.05
1379.59
1330.28
1251.94
1225.24
1203.32
1159.37
1082.50
1029.31
1015.21
968.15
935.53
906.55
807.21
761.48
718.57
679.16
637.03
573.50
515.63
496.23
434.88
395.86
349.45
332.86
323.16
0.0
0.1
0.2
0.3
0.4
0.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Eu(1,7-Medo2ampa)]

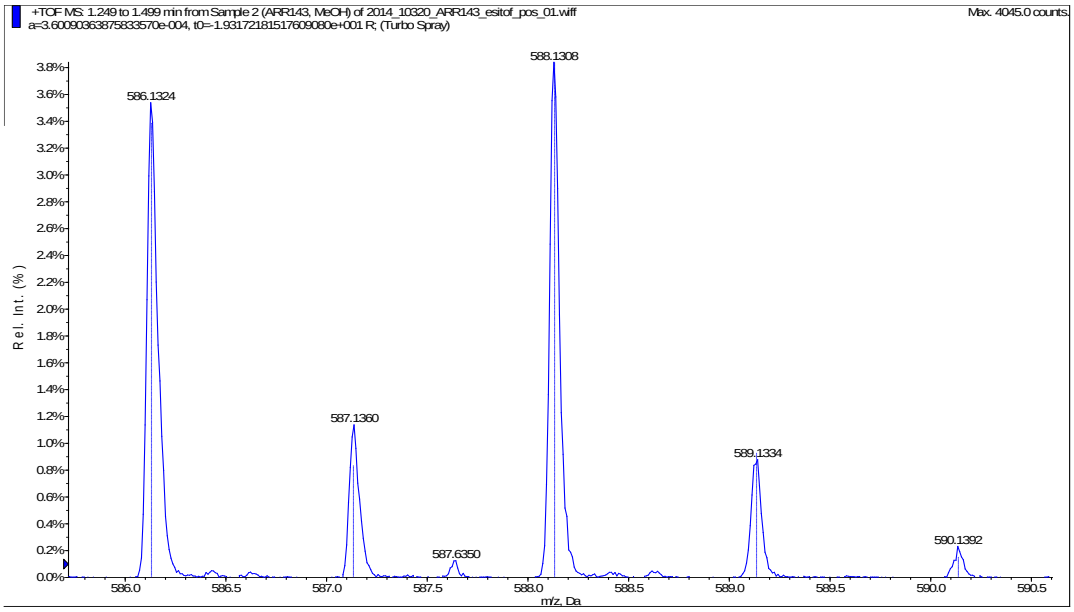
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



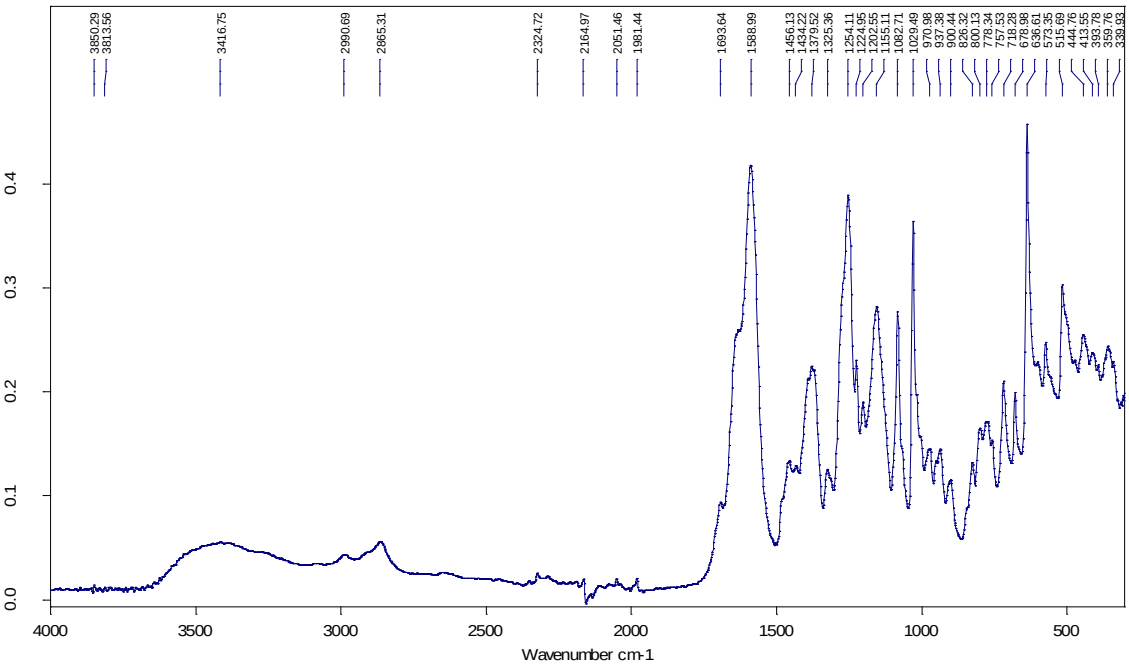
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

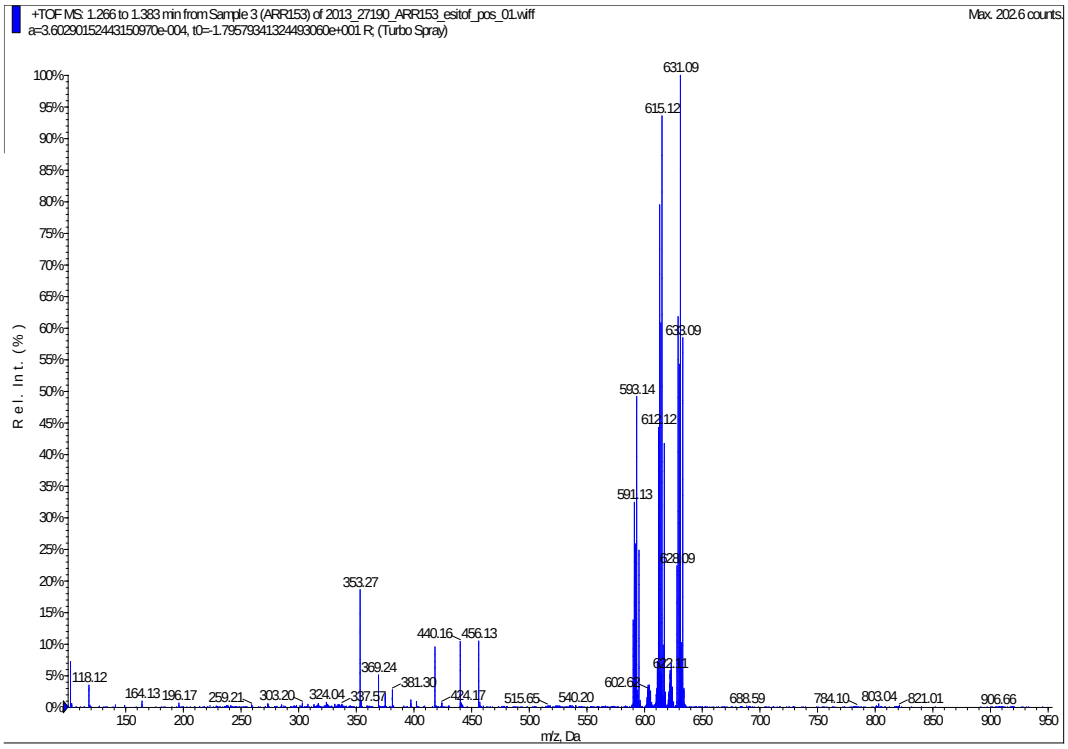


Espectro IR

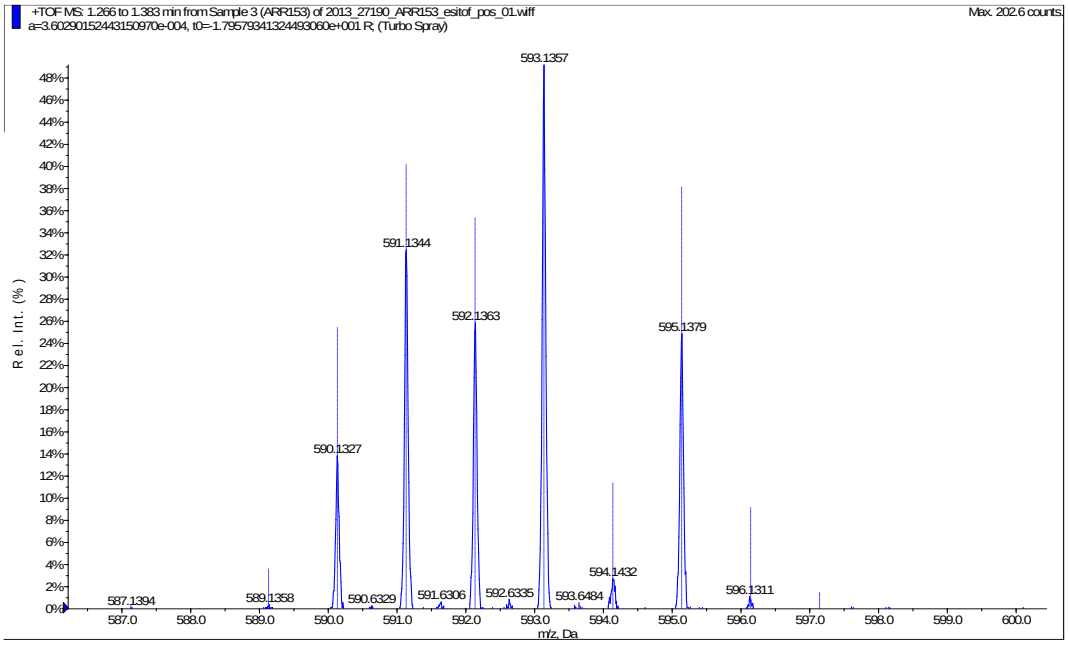


[Gd(1,7-Medo2ampa)]

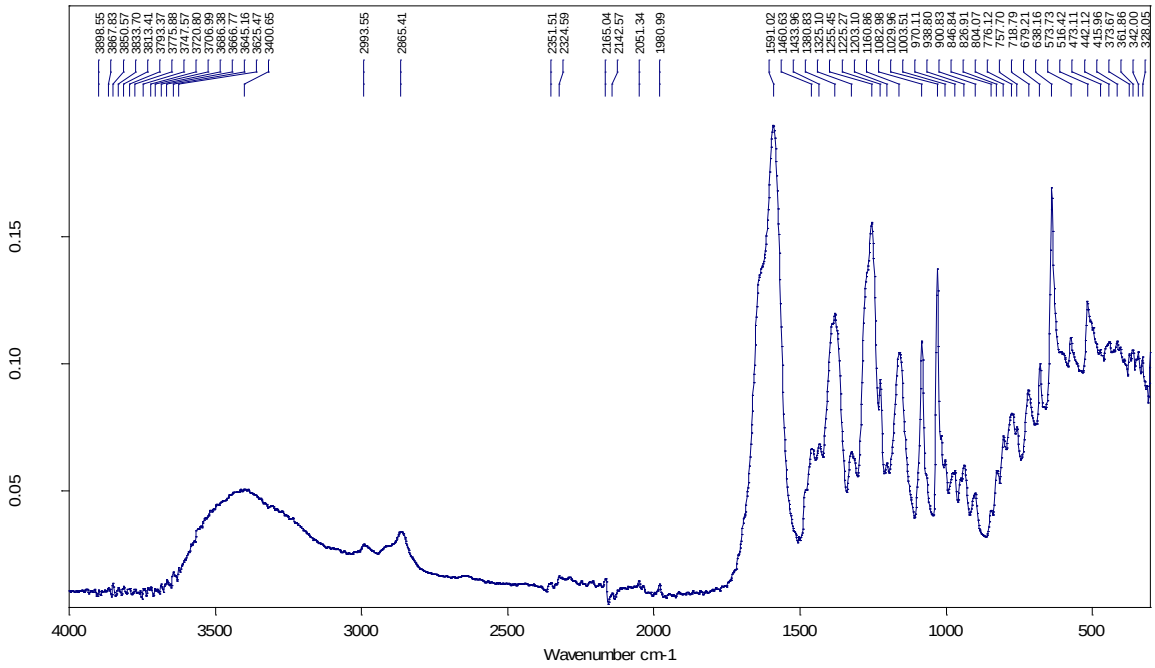
Espectro de masas ESI+



Espectro ESI+ HR

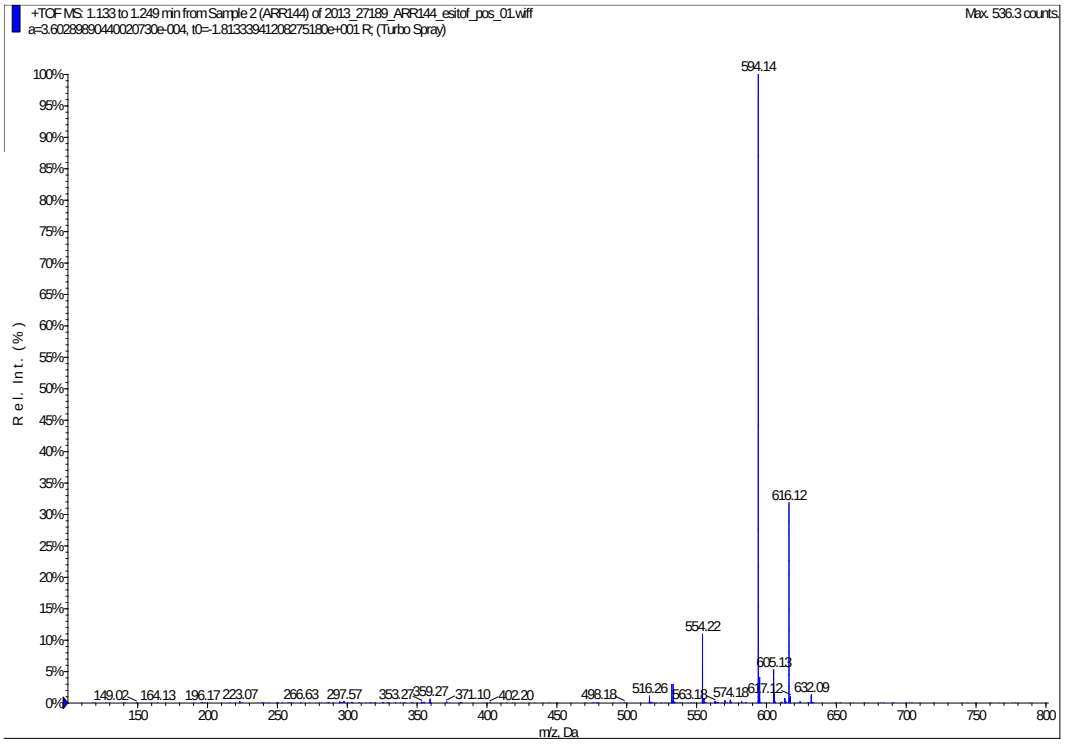


Espectro IR

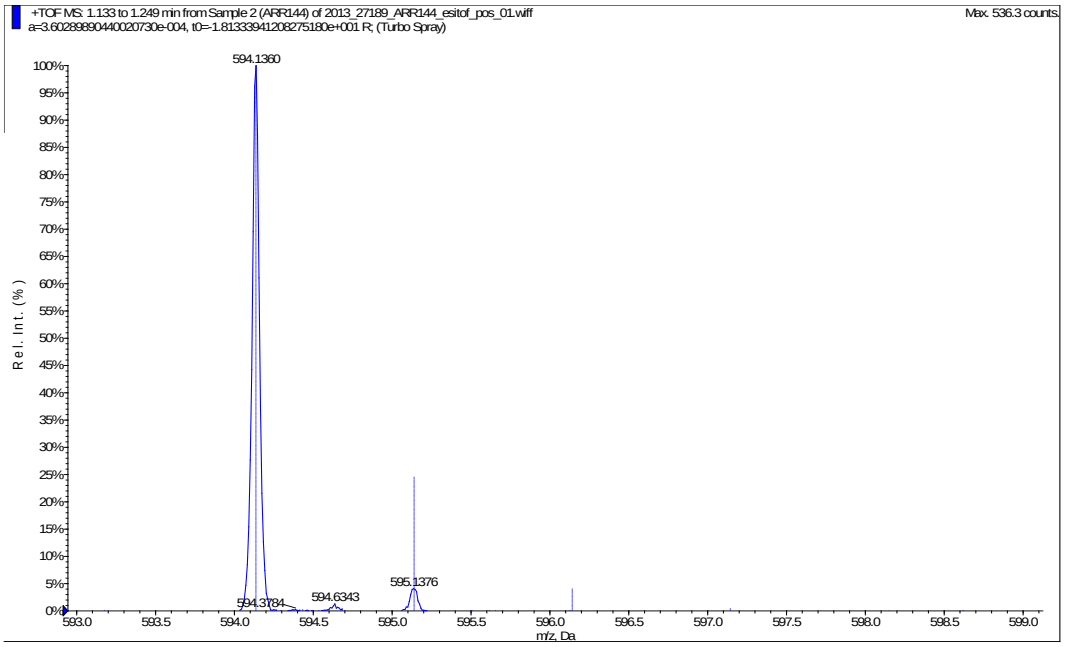

3898.55
3867.83
3850.57
3833.70
3813.41
3793.37
3775.88
3747.57
3720.80
3706.99
3686.38
3666.77
3645.16
3625.47
3400.65
2993.55
2865.41
2351.51
2324.59
2165.04
2142.57
2051.34
1980.99
1591.02
1460.63
1433.96
1380.83
1325.10
1225.45
1225.27
1203.10
1160.86
1082.98
1029.96
1003.51
970.11
938.60
900.83
846.84
826.91
804.07
776.12
757.70
718.29
679.21
638.16
573.73
516.42
473.11
442.12
415.96
377.67
361.86
342.00
328.05
0.15
0.10
0.05
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(1,7-Medo2ampa)]

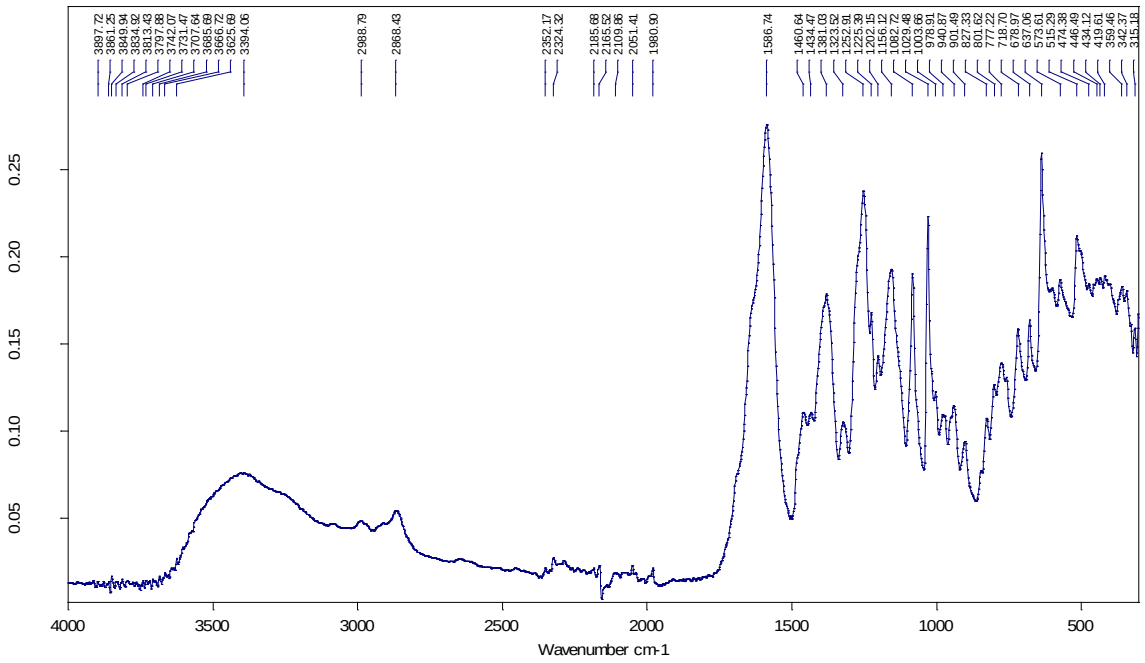
Espectro de masas ESI+



Espectro ESI+ HR

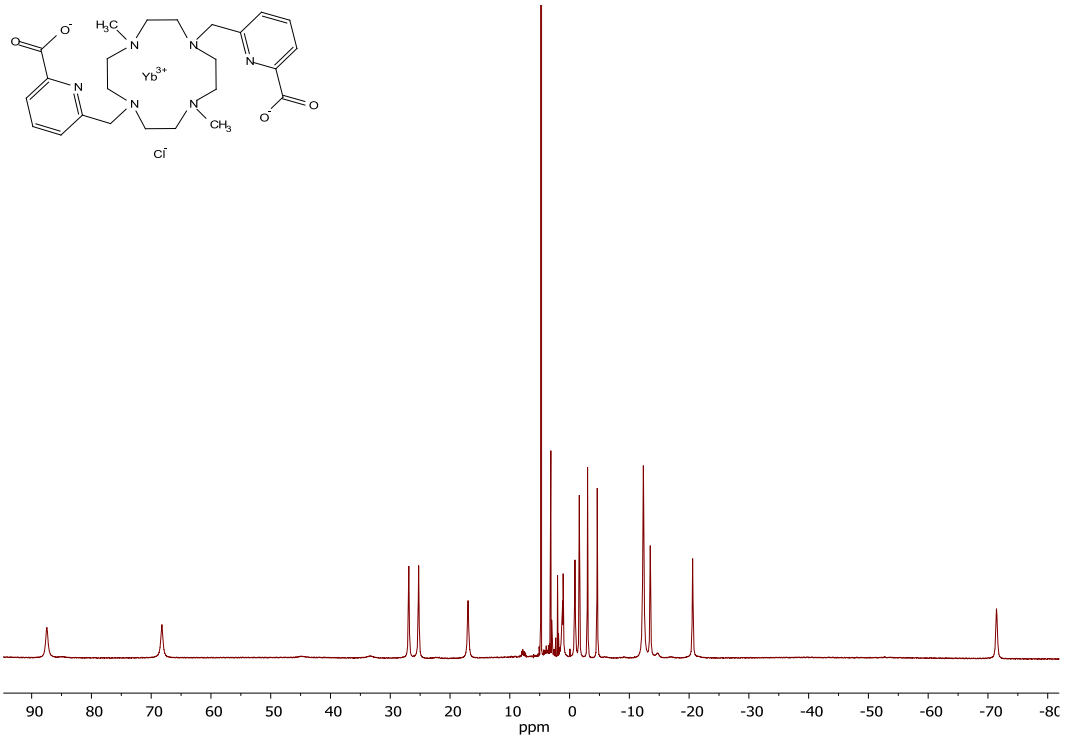


Espectro IR

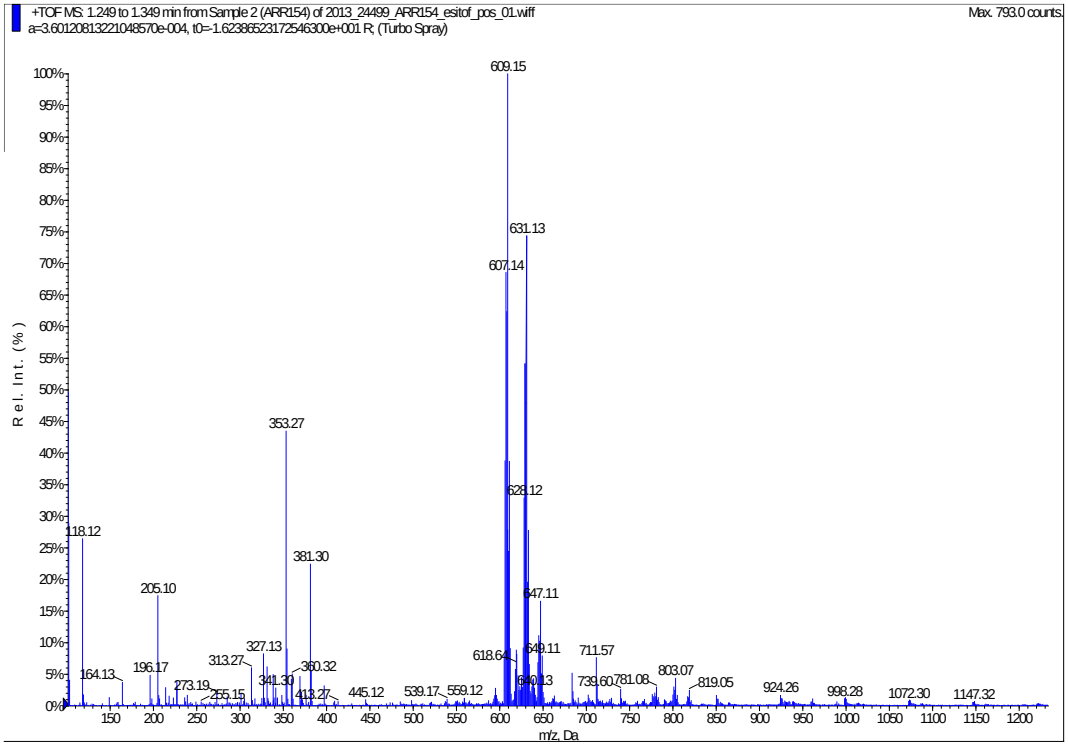

3897.72
3861.25
3849.94
3824.92
3813.43
3797.88
3742.07
3731.47
3707.64
3665.69
3645.72
3625.69
3394.06
2968.79
2868.43
2352.17
2324.32
2185.68
2165.52
2109.86
2051.41
1980.90
1586.74
1460.64
1434.47
1381.03
1321.52
1252.91
1225.39
1202.15
1156.12
1082.72
1023.48
1003.65
978.91
940.87
901.49
827.33
801.62
777.22
713.70
678.97
637.06
573.61
515.29
474.38
446.49
434.12
419.61
359.46
342.37
315.18
0.25
0.20
0.15
0.10
0.05
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Yb(1,7-Medo2ampa)]

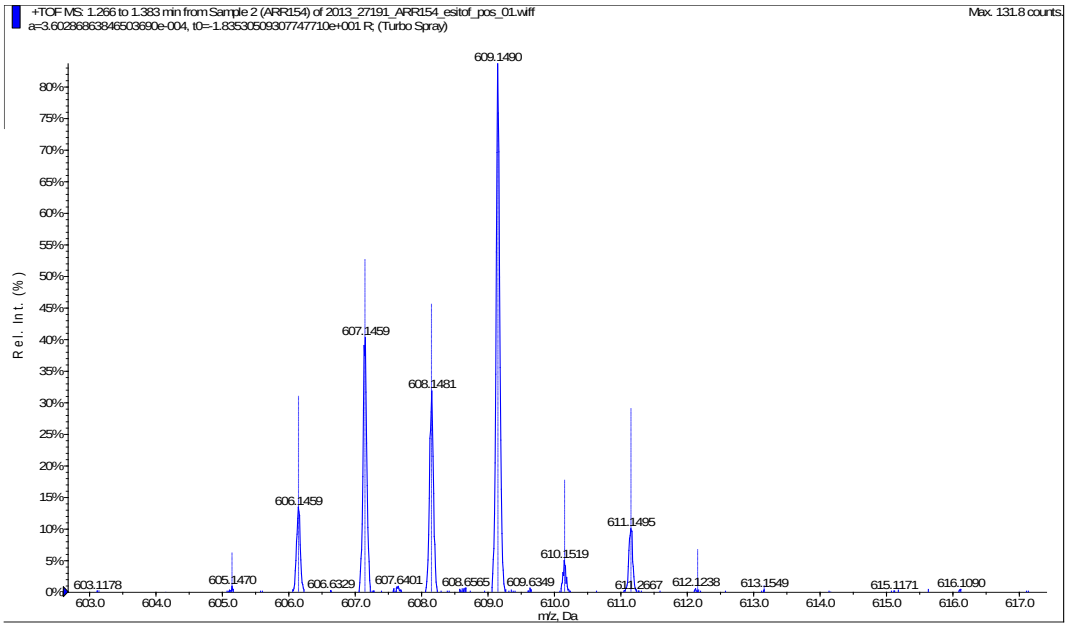
^{1}H-RMN (D_2O, 278K, 500 MHz) (δ/ppm)



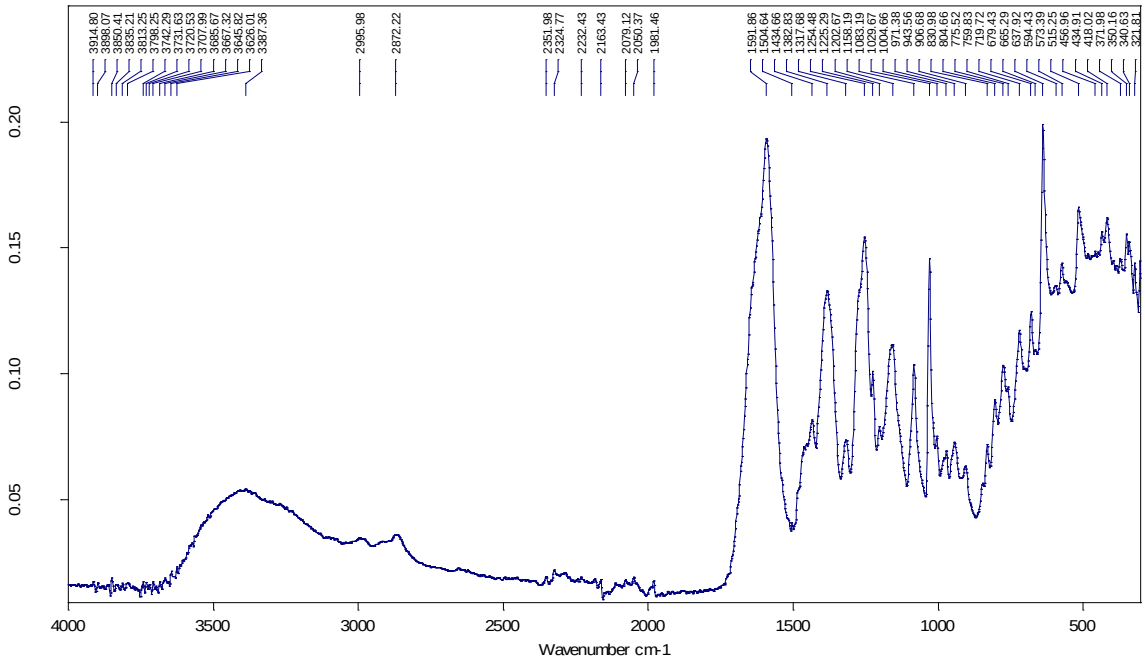
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

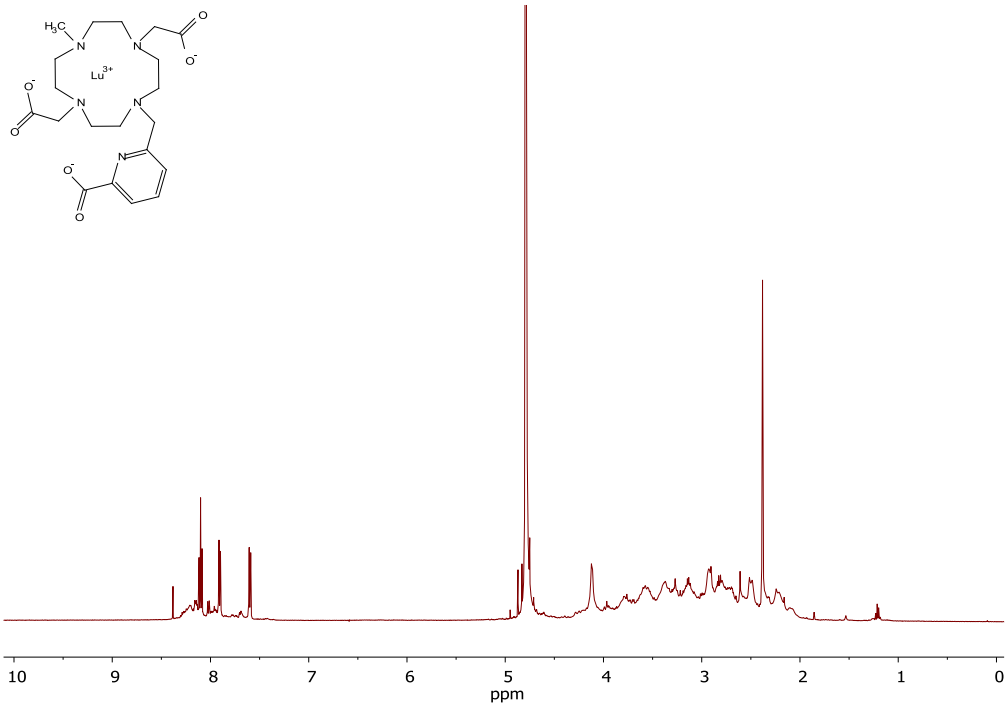


Espectro IR

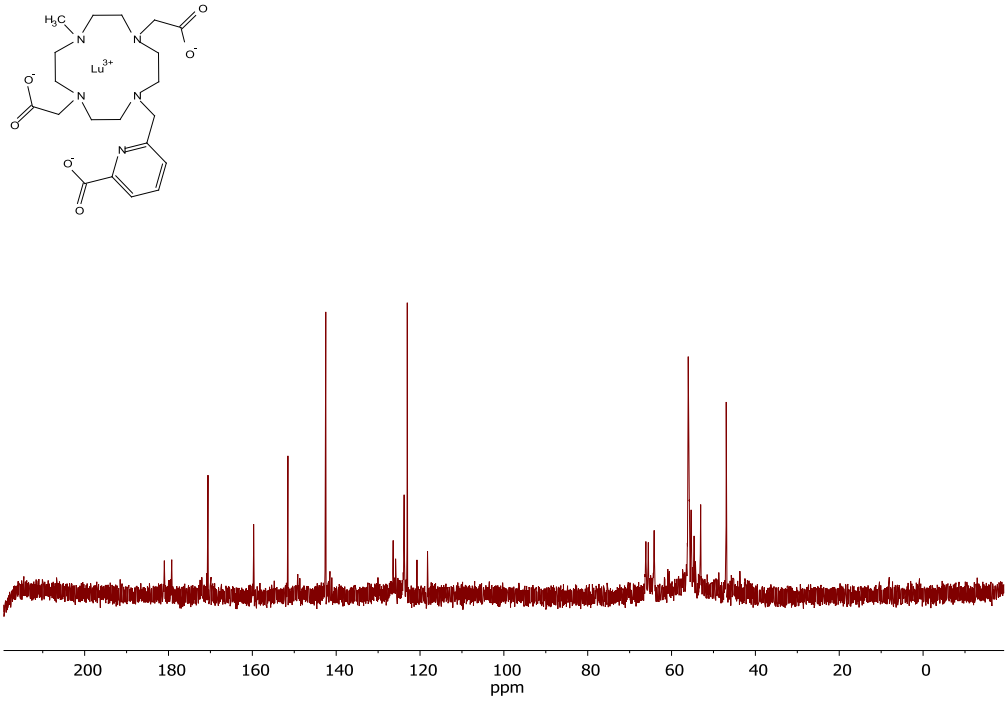


[Lu(1,7-Medo2ampa)]

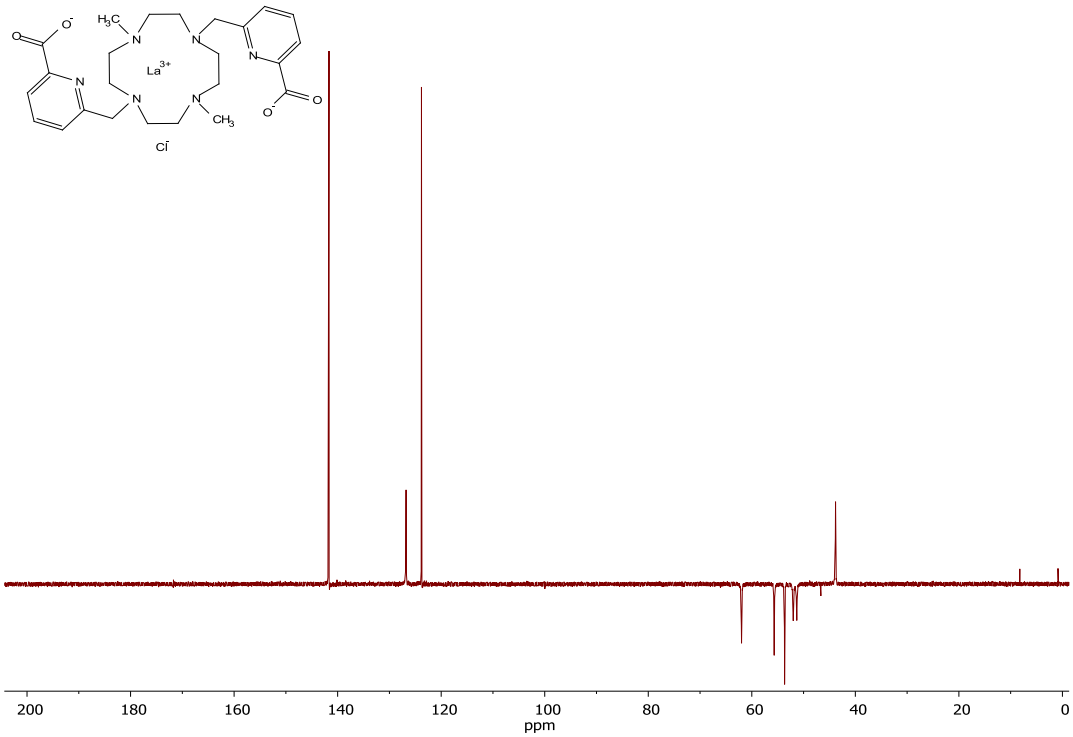
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



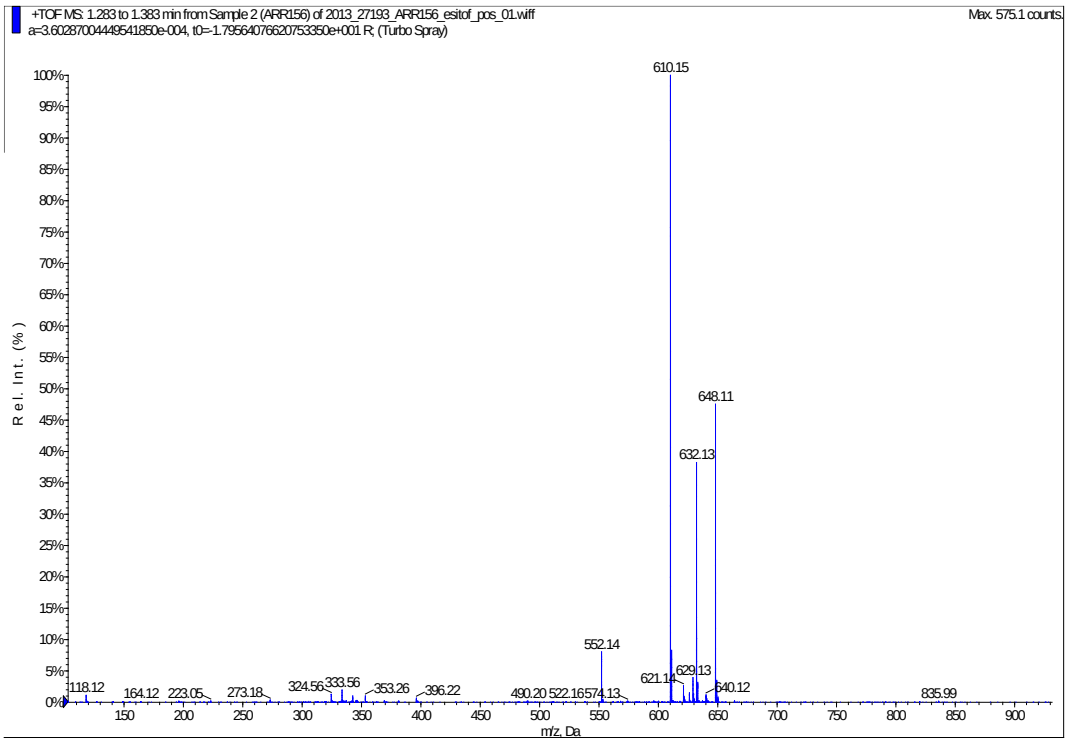
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



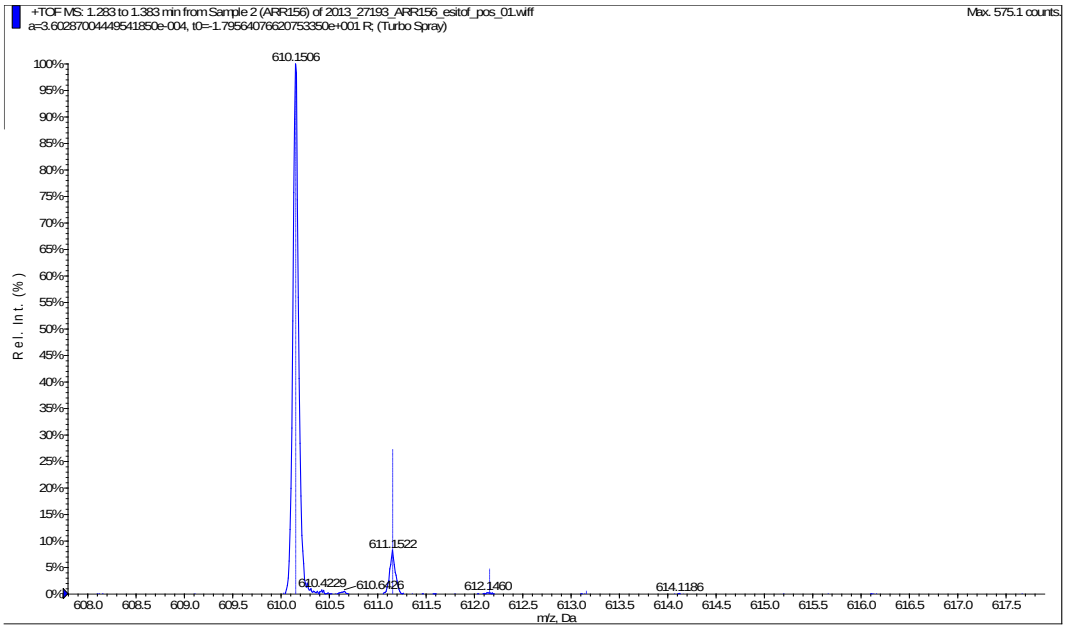
DEPT-RMN (D_2O) (δ/ppm)



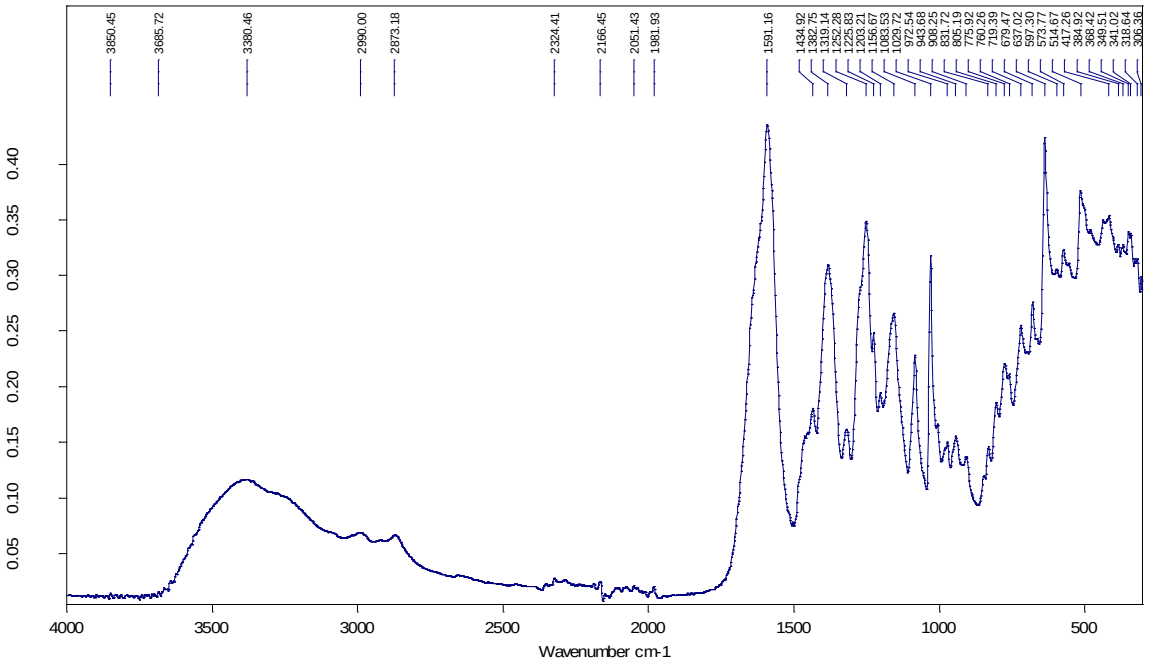
Espectro de masas ESI^+



Espectro ESI⁺ HR

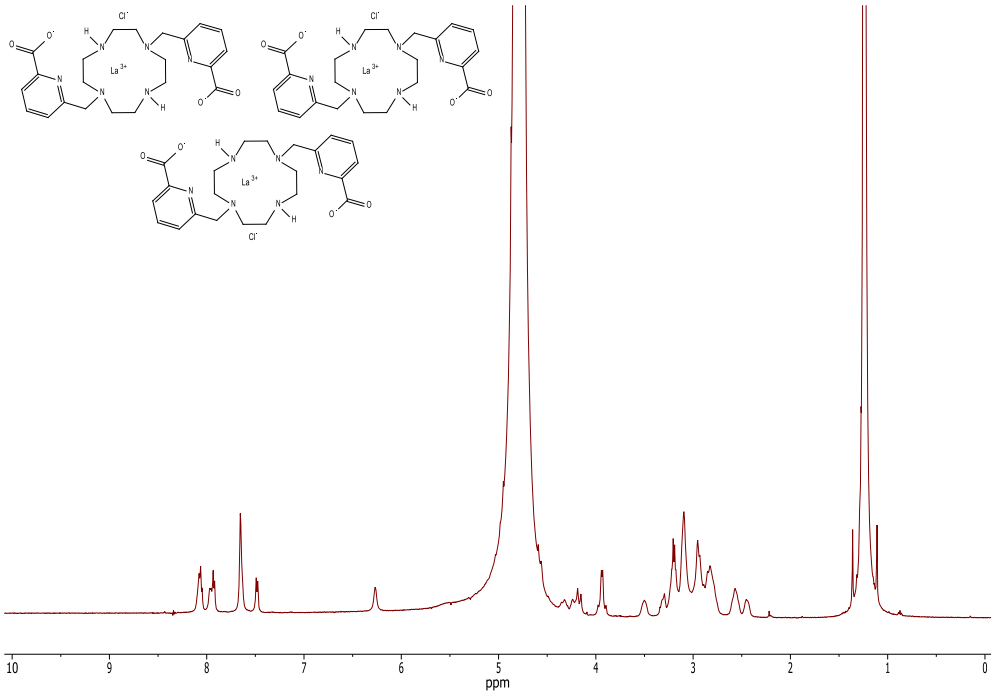


Espectro IR

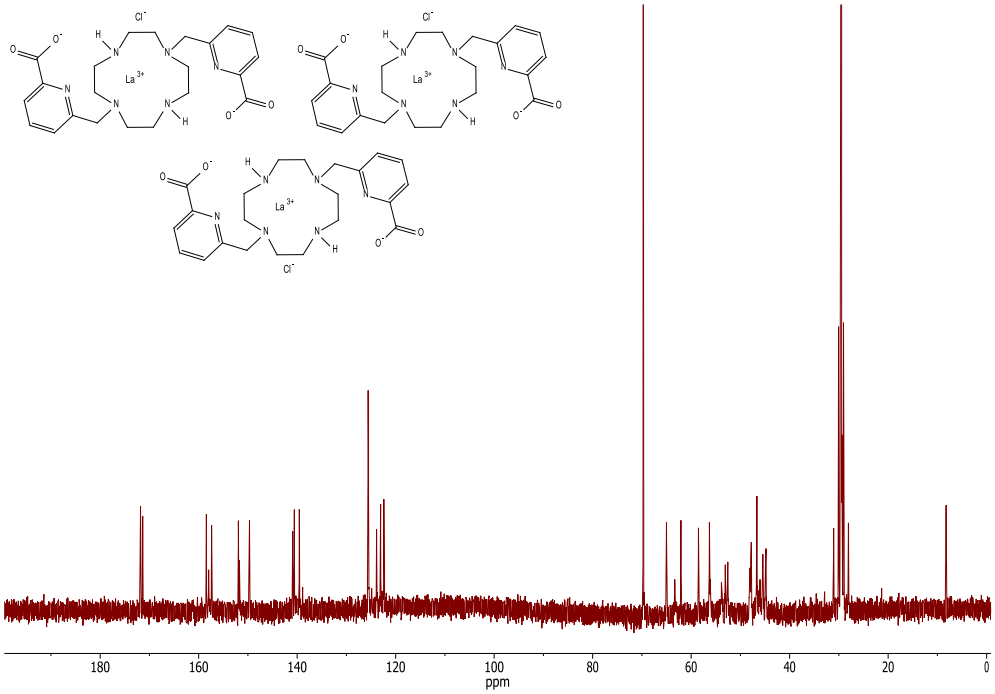


[La(dodpa)]Cl

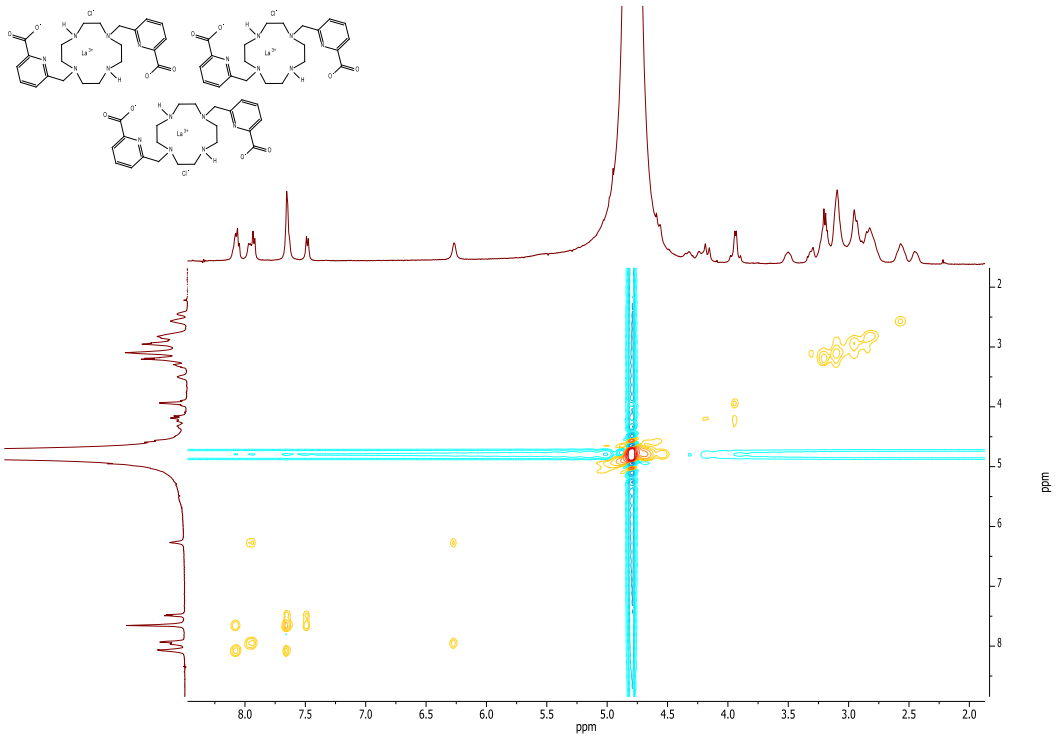
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



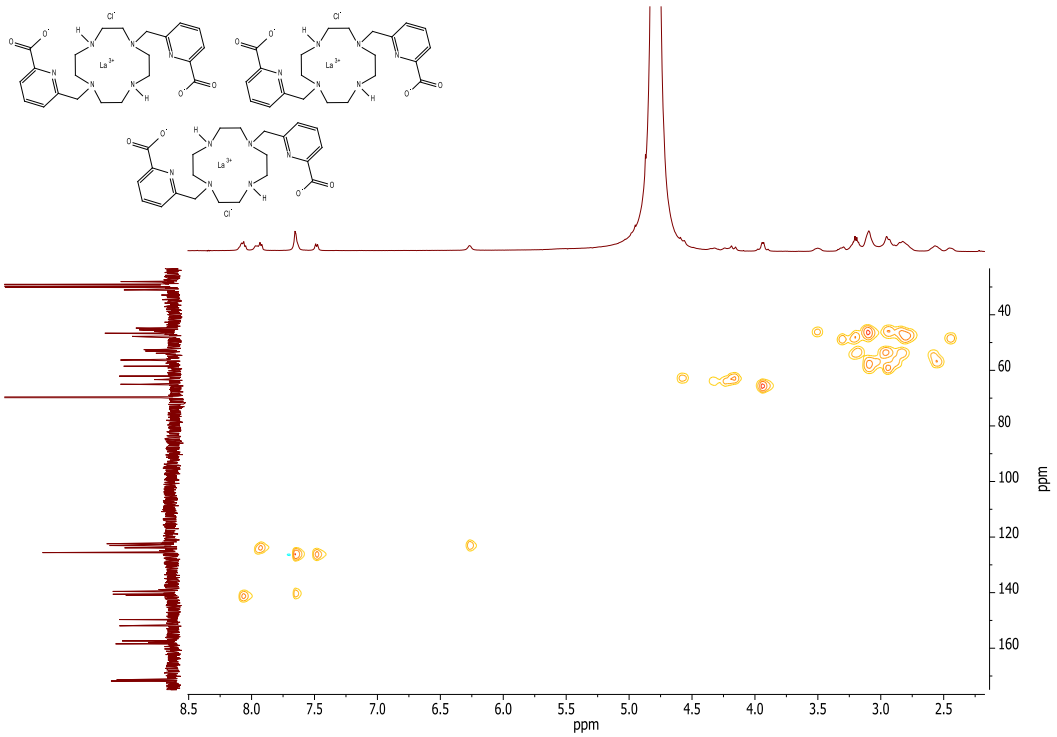
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



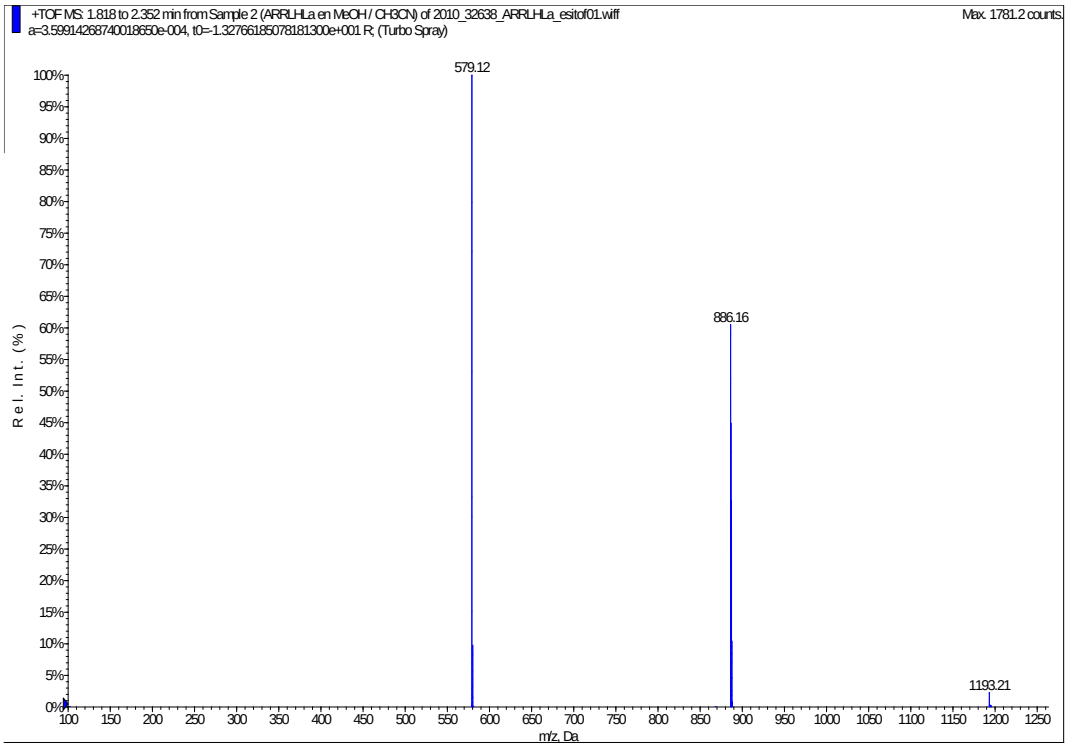
COSY-RMN (D_2O) (δ/ppm)



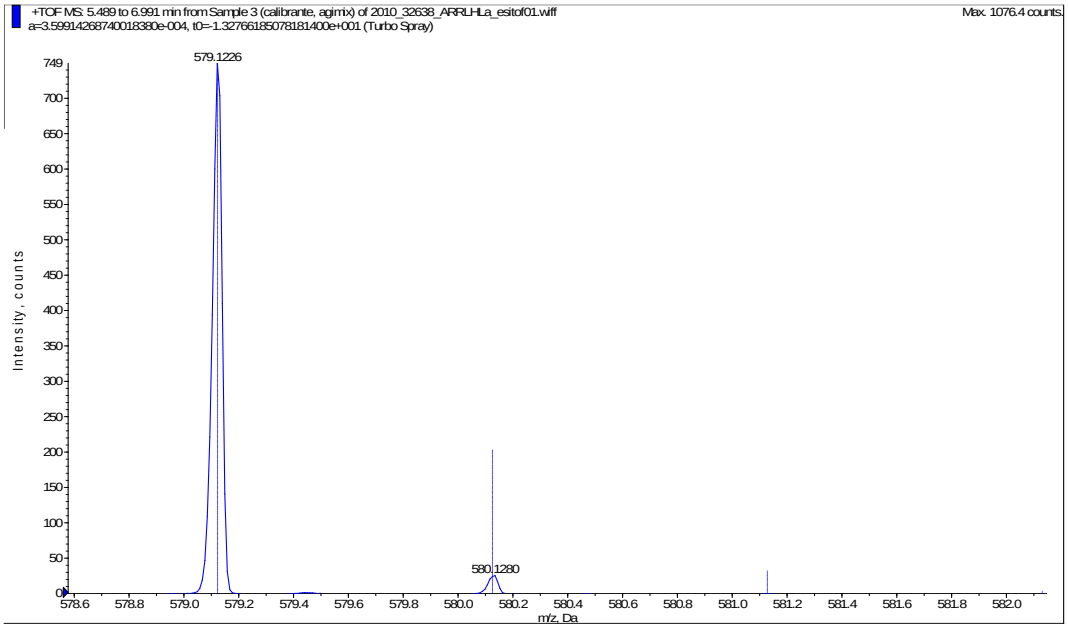
HSQC-RMN (D_2O) (δ/ppm)



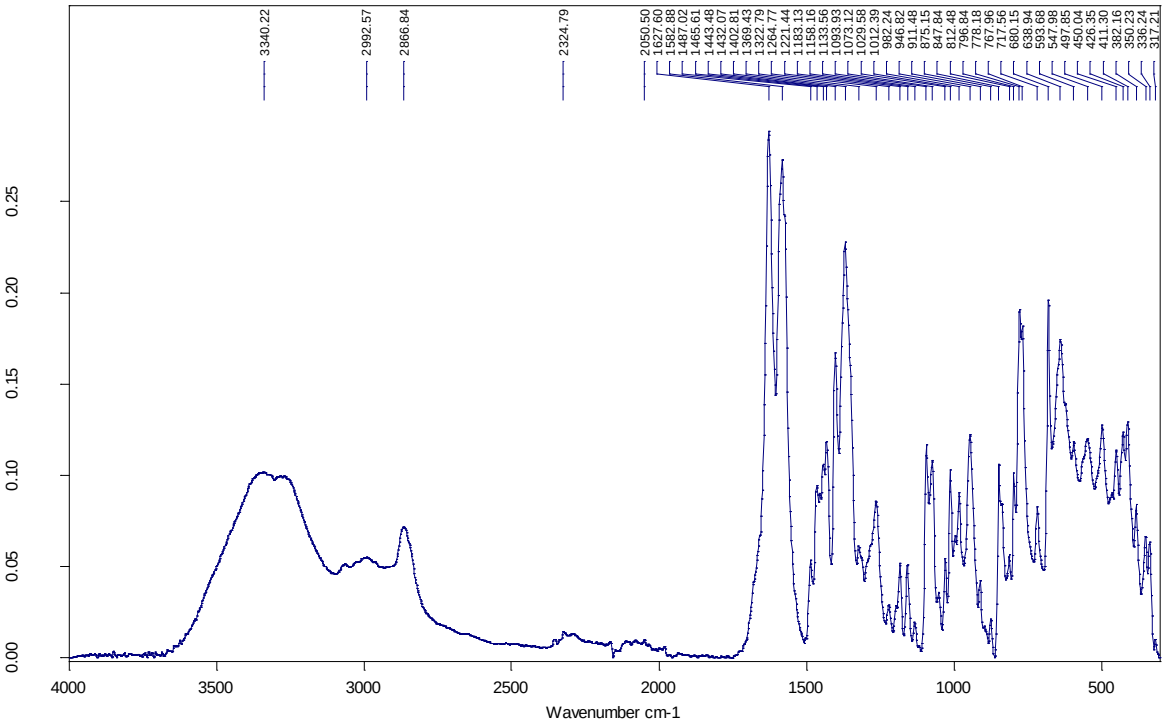
Espectro de masas ESI+



Espectro ESI+ HR

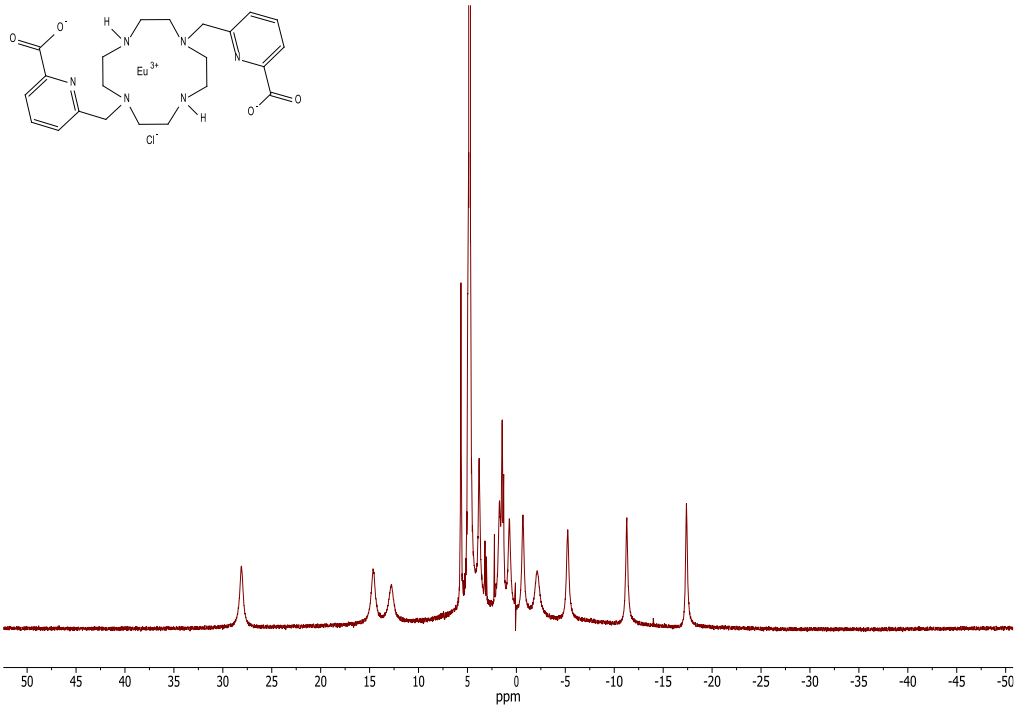


Espectro IR

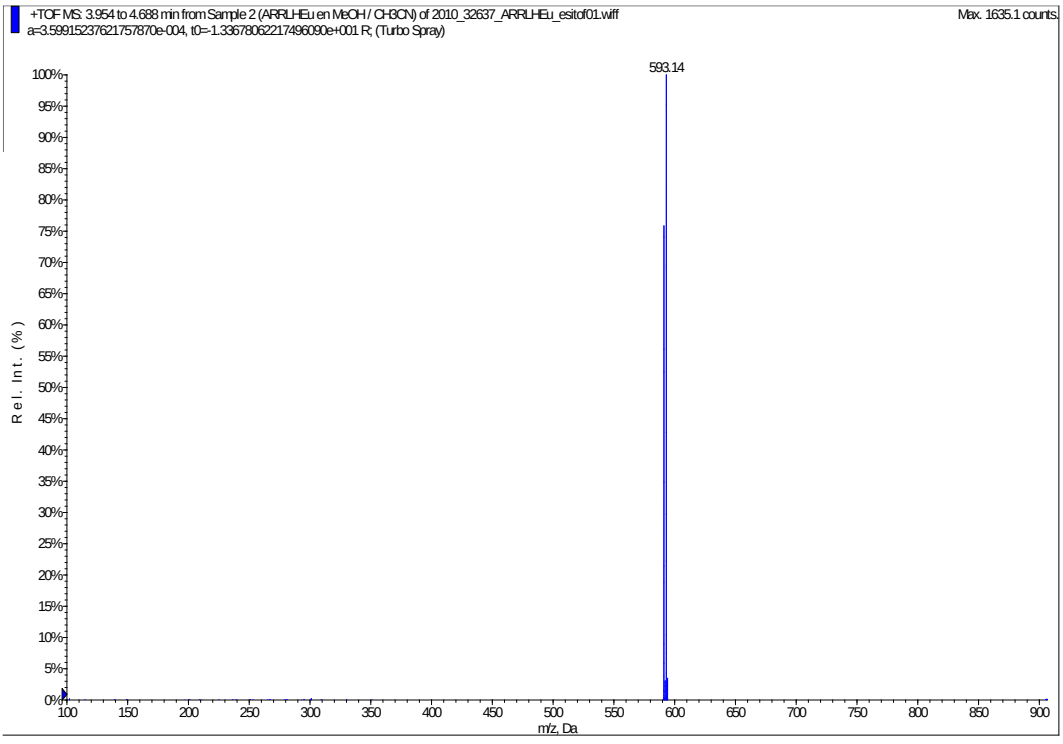

3340.22
2992.57
2866.84
2324.79
2050.50
1627.60
1582.88
1487.02
1465.61
1443.48
1432.07
1402.81
1369.43
1322.79
1264.77
1221.44
1183.13
1158.16
1133.96
1093.93
1073.22
1029.58
1012.39
982.24
946.82
911.48
875.15
847.84
812.48
796.84
779.18
757.96
717.56
680.15
638.94
593.68
547.98
497.85
450.04
426.35
411.30
382.16
362.23
336.24
317.21
0.00
0.05
0.10
0.15
0.20
0.25
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Eu(dodpa)]Cl

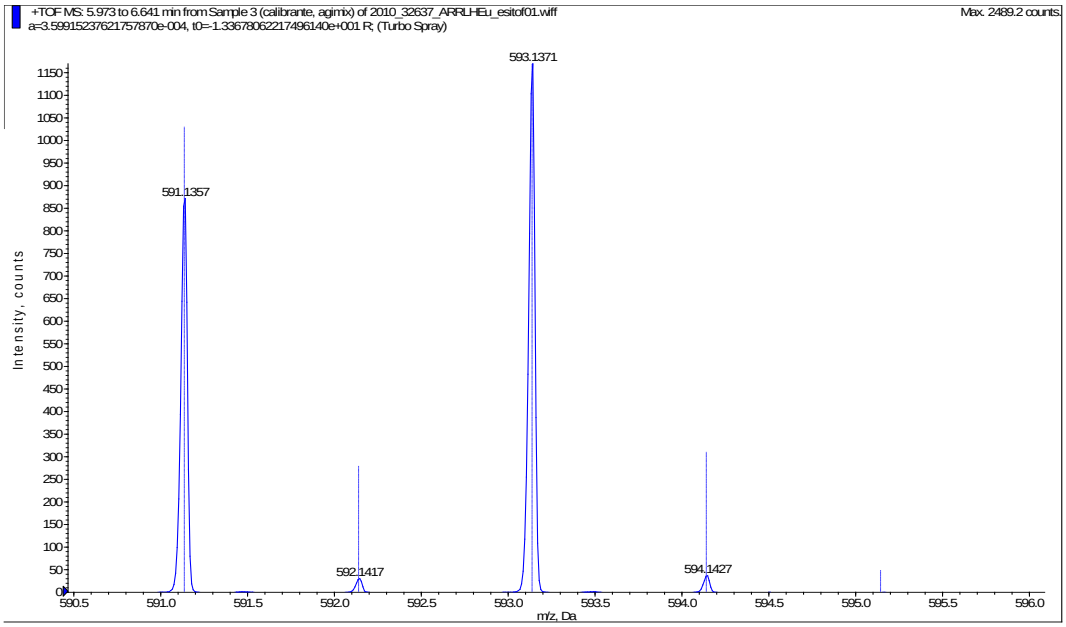
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



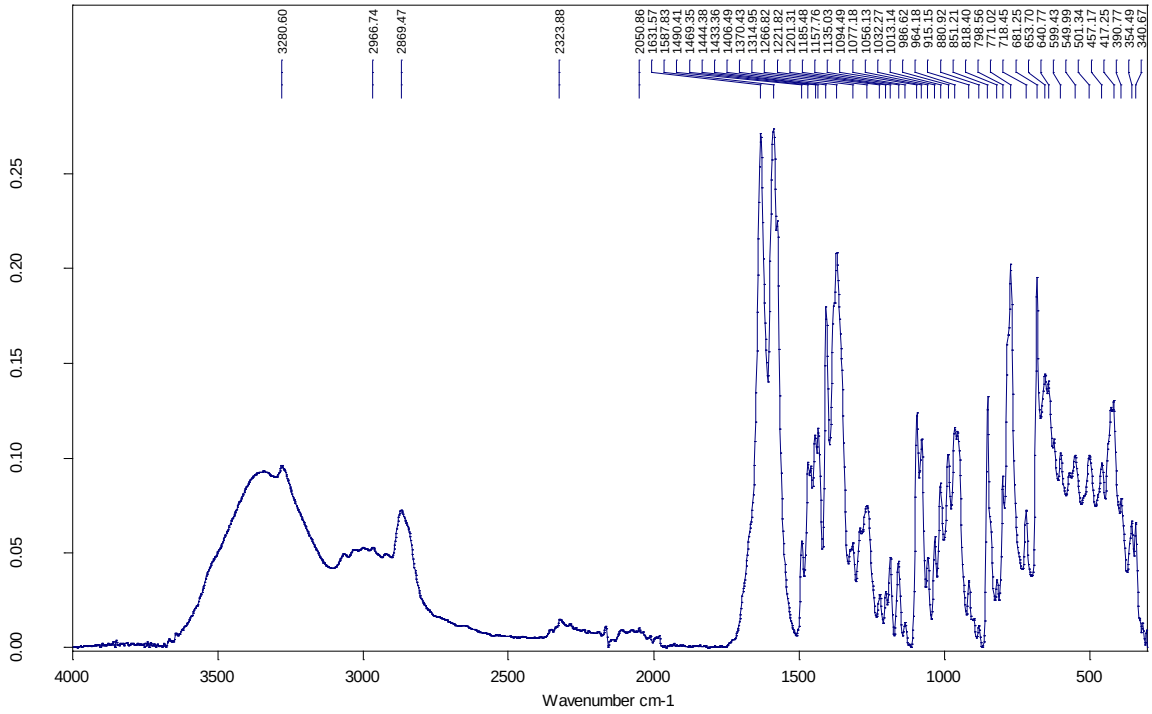
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

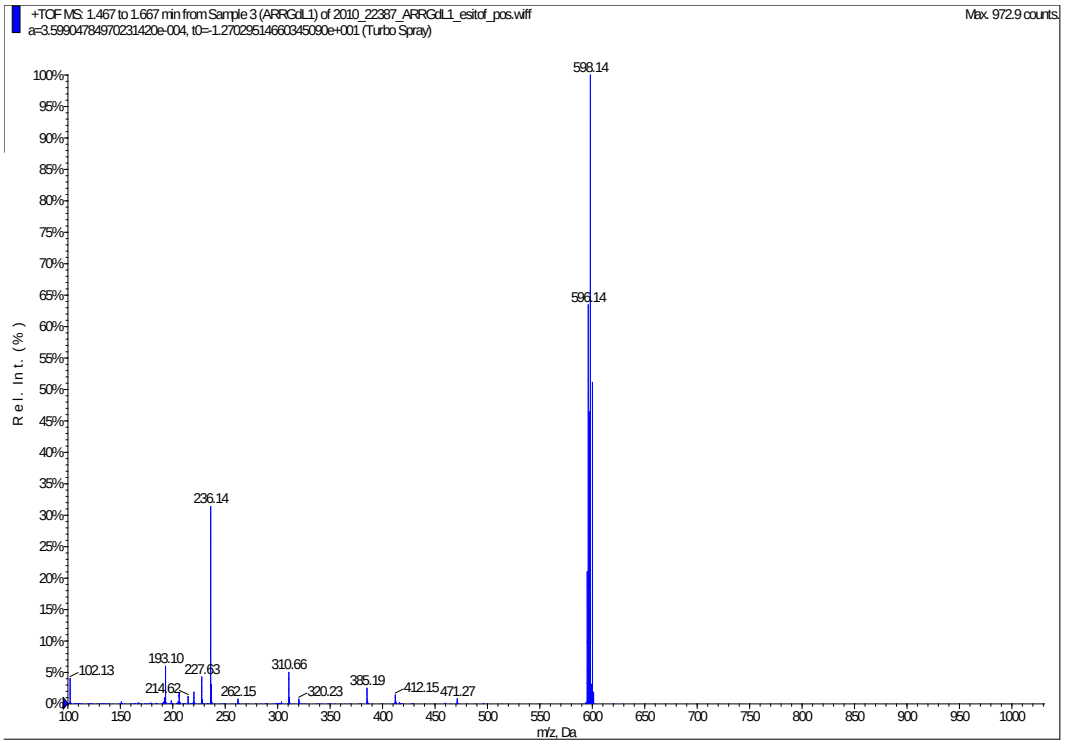


Espectro IR

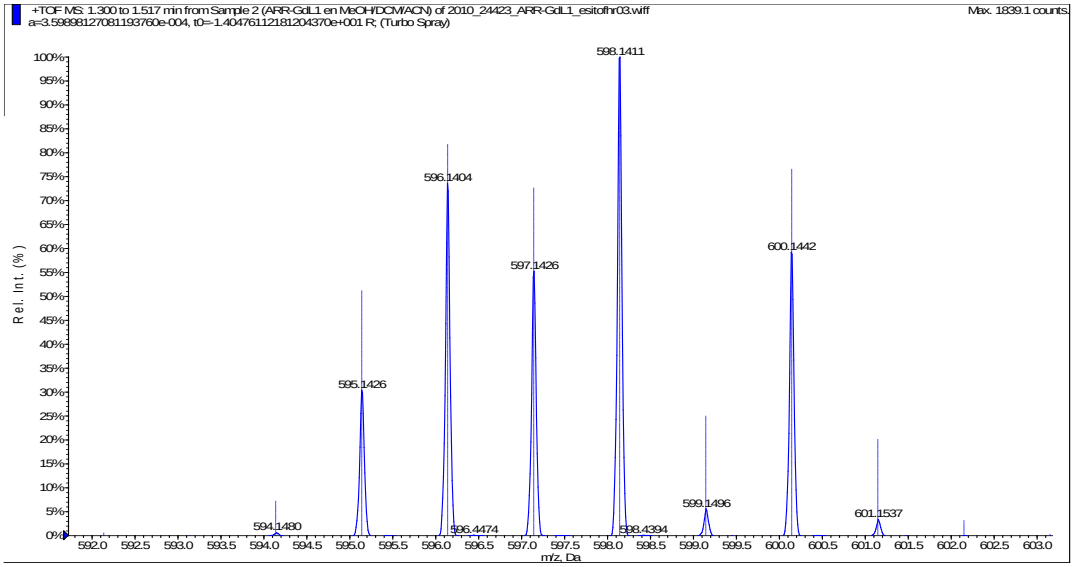


[Gd(dodpa)]Cl

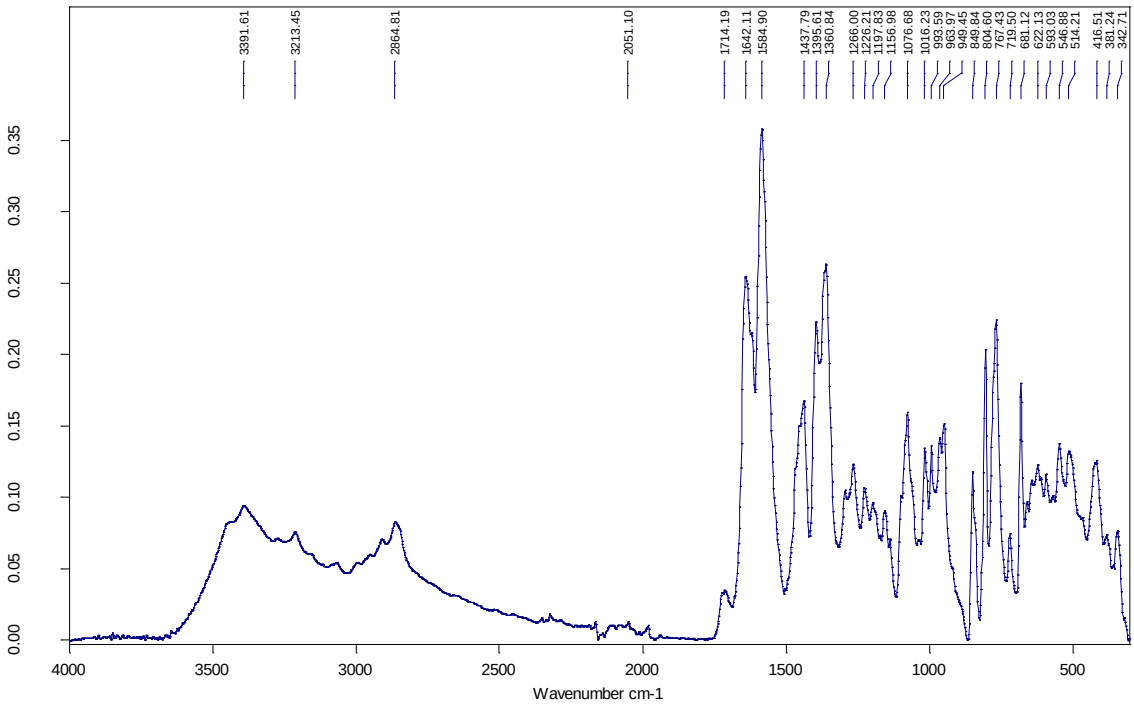
Espectro de masas ESI+



Espectro ESI+ HR

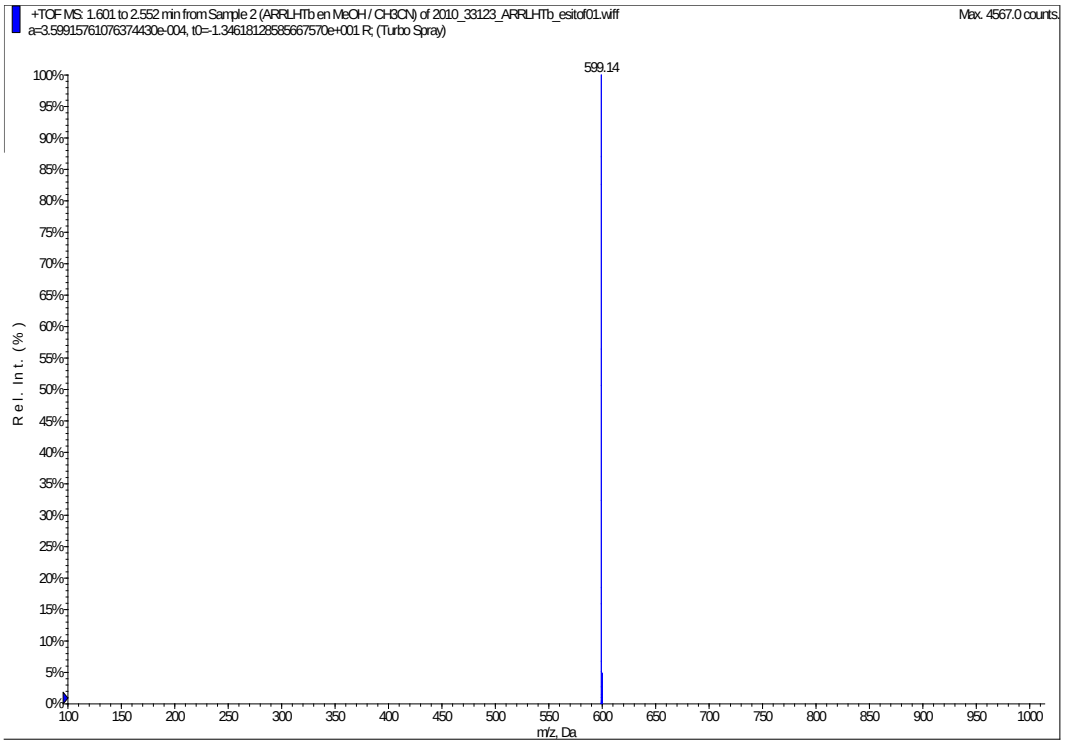


Espectro IR

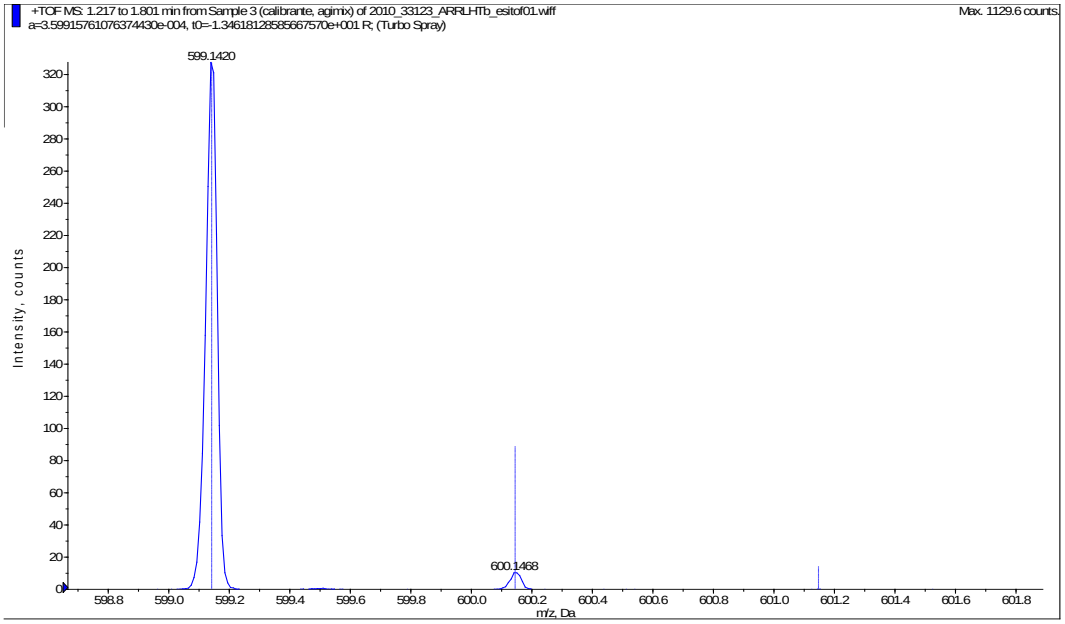

3391.61
3213.45
2864.81
2051.10
1714.19
1642.11
1584.90
1437.79
1395.61
1360.84
1266.00
1226.21
1197.83
1156.98
1076.68
1016.23
993.59
967.07
949.45
849.84
804.60
767.43
719.50
681.12
622.13
593.03
546.88
514.21
416.51
381.24
342.71
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(dodpa)]Cl

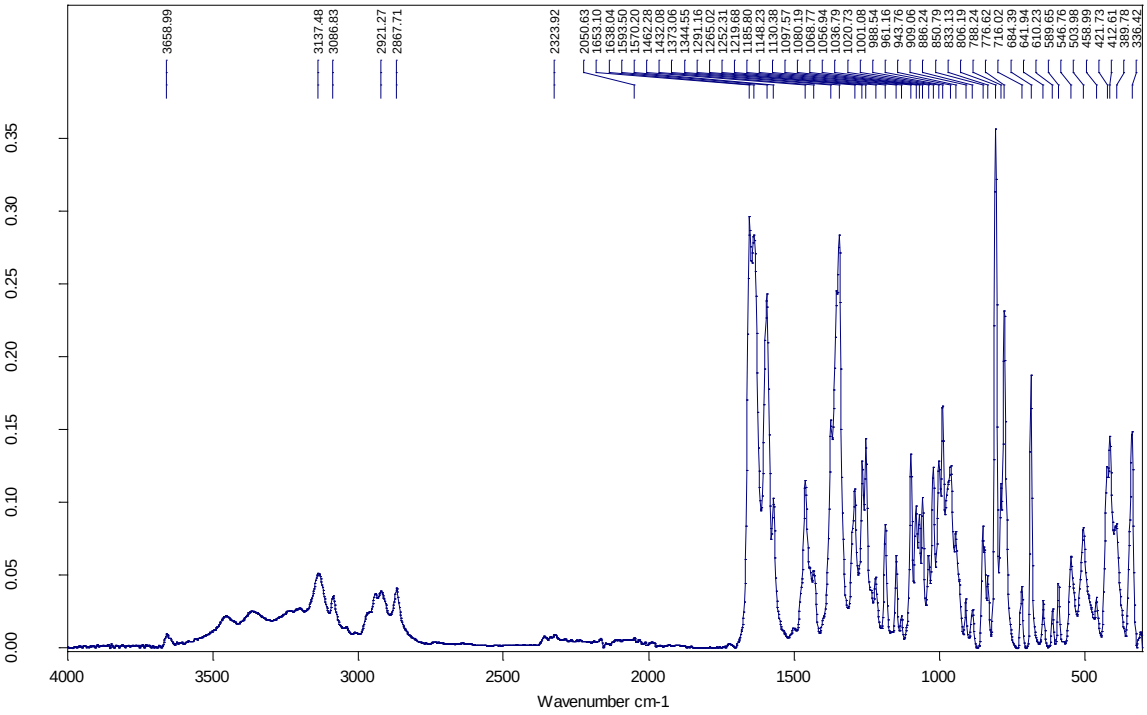
Espectro de masas ESI+



Espectro ESI+ HR

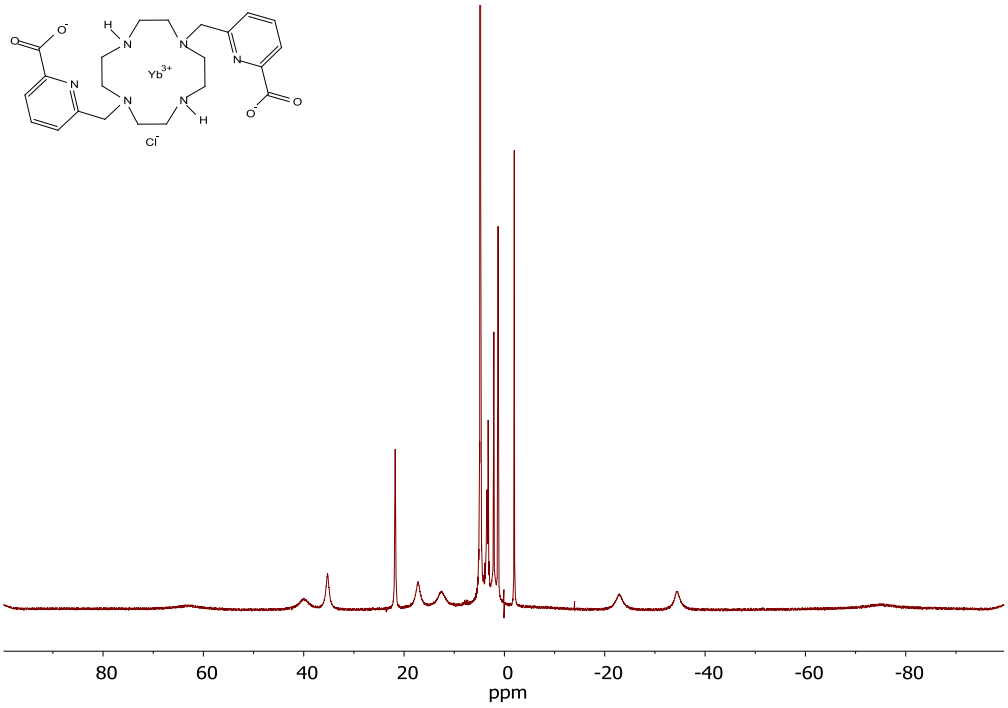


Espectro IR

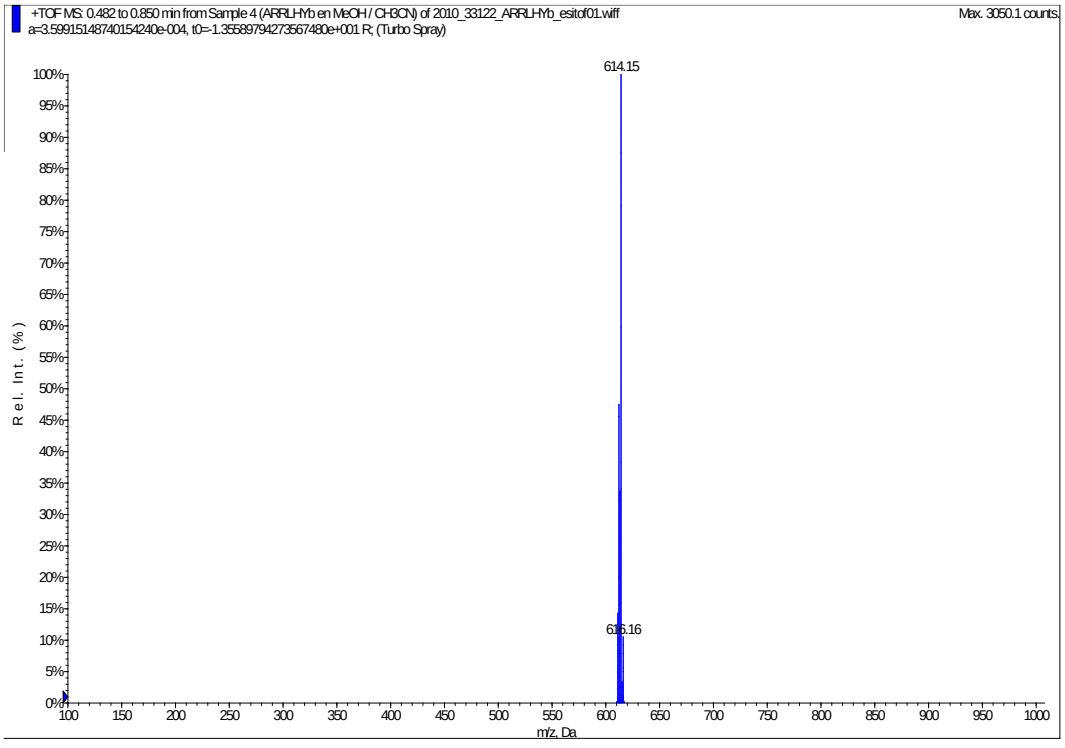

3658.99
3137.48
3086.83
2921.27
2867.71
2323.92
2050.63
1653.10
1598.04
1570.20
1462.28
1432.08
1373.06
1344.55
1291.16
1265.02
1252.31
1219.68
1185.80
1148.23
1130.38
1097.57
1080.19
1068.77
1056.94
1036.79
1020.73
1001.08
988.54
961.16
943.76
909.06
886.24
850.79
833.13
806.19
793.24
776.62
716.02
684.39
641.94
610.23
589.65
546.76
503.98
458.99
427.73
412.61
389.78
336.42
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Yb(dodpa)]Cl

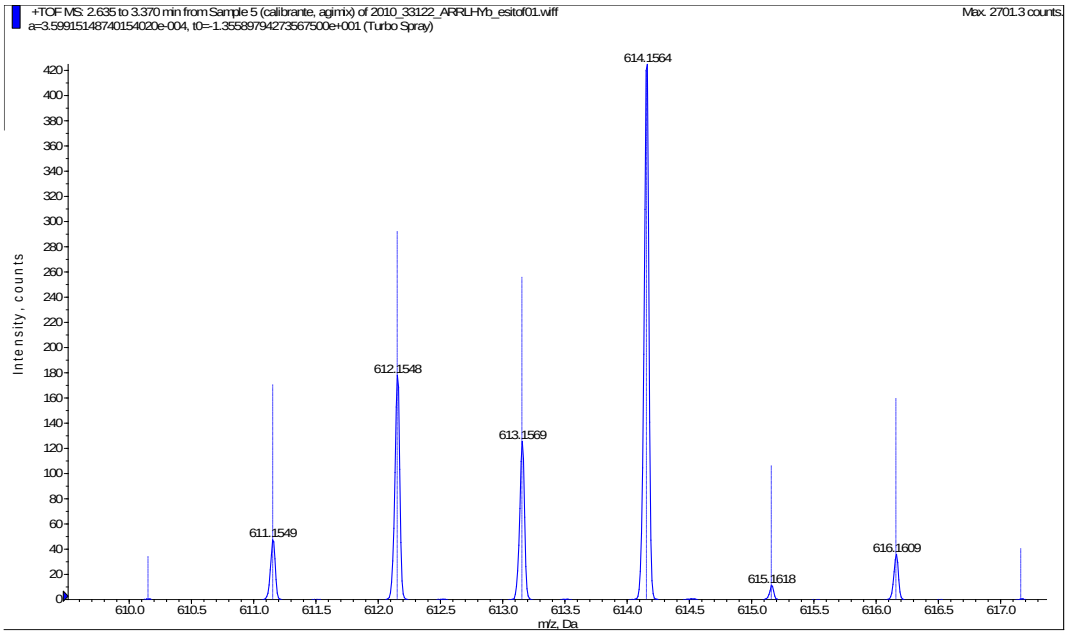
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



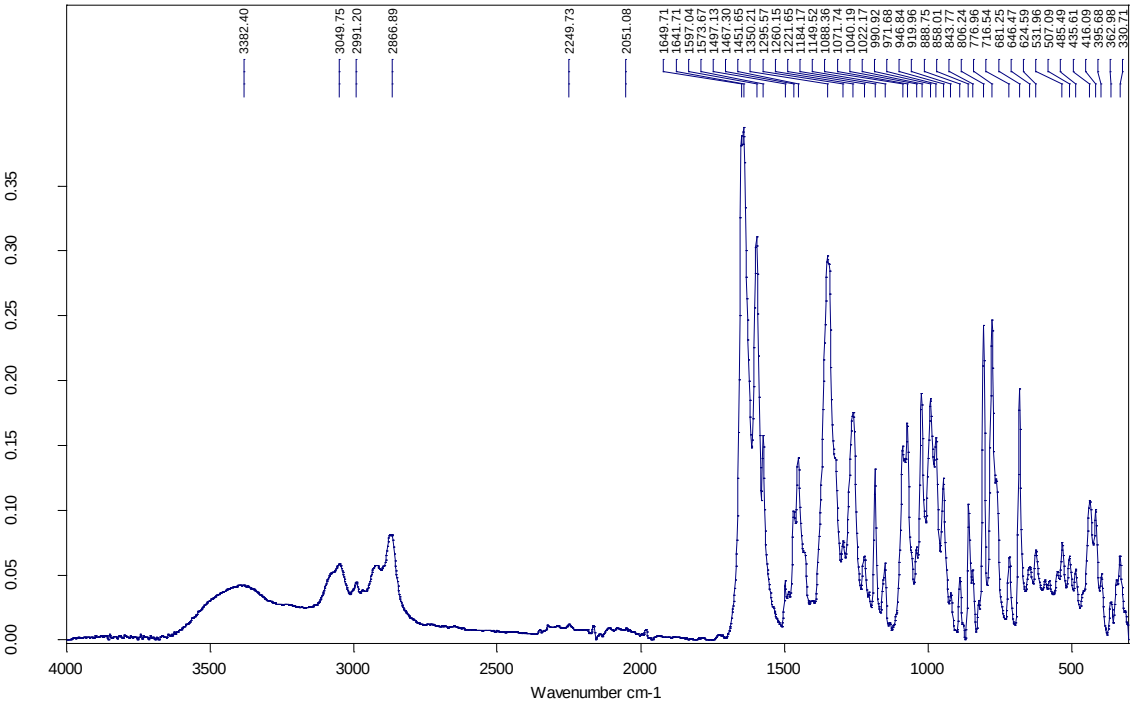
Espectro de masas ESI$^+$



Espectro ESI+ HR

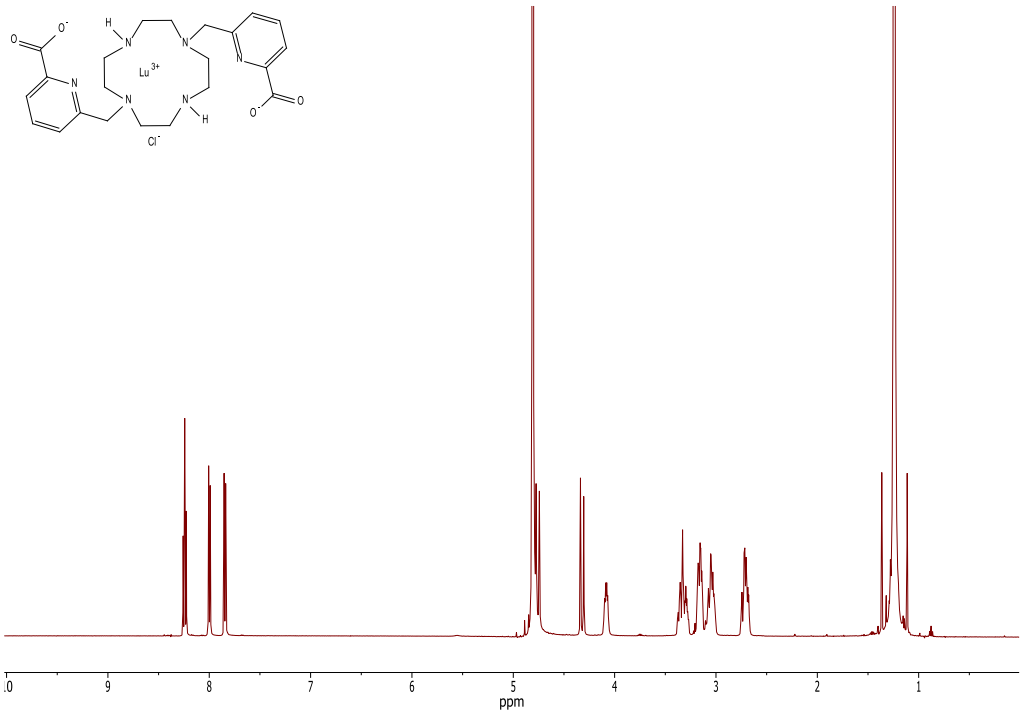


Espectro IR

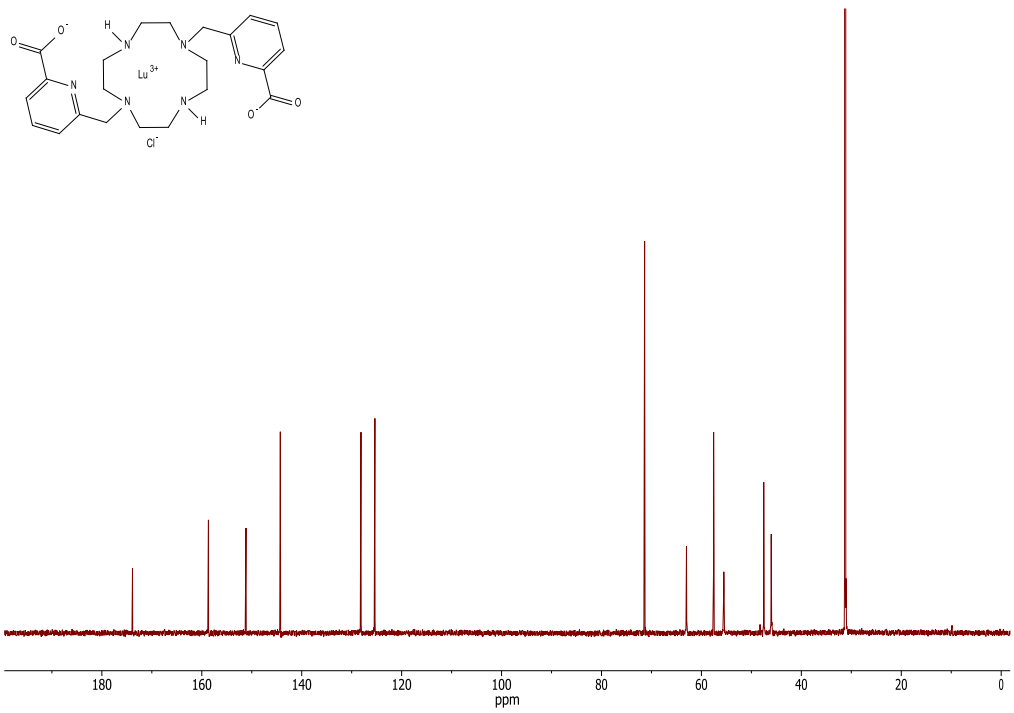


[Lu(dodpa)]Cl

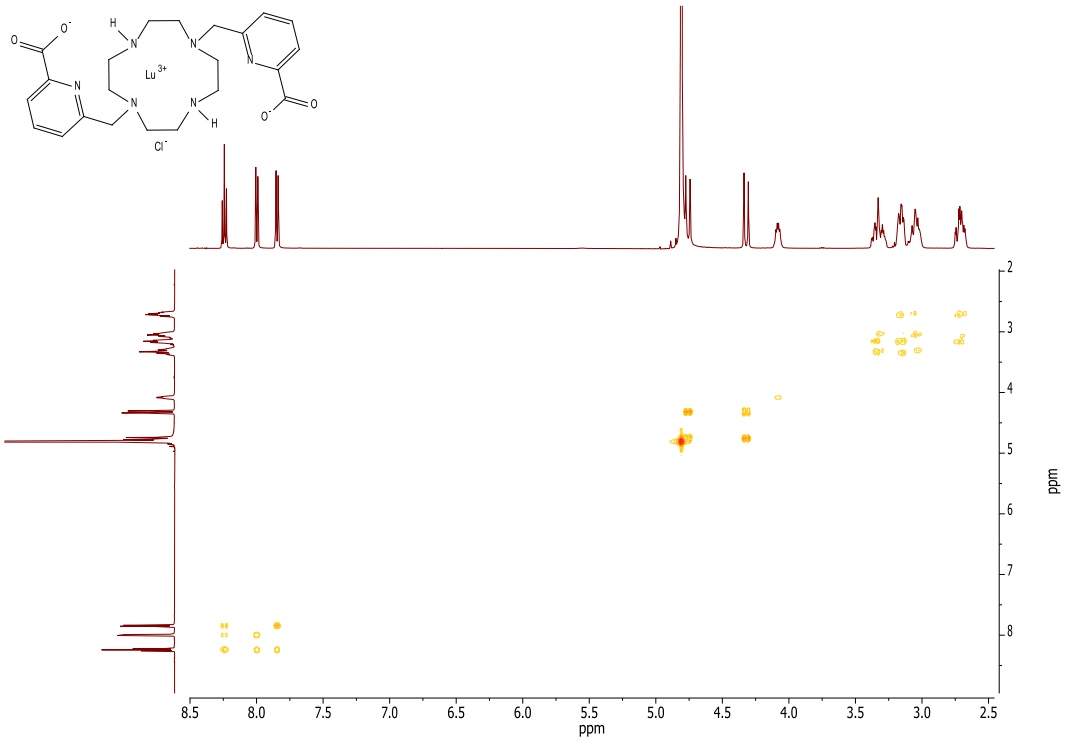
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



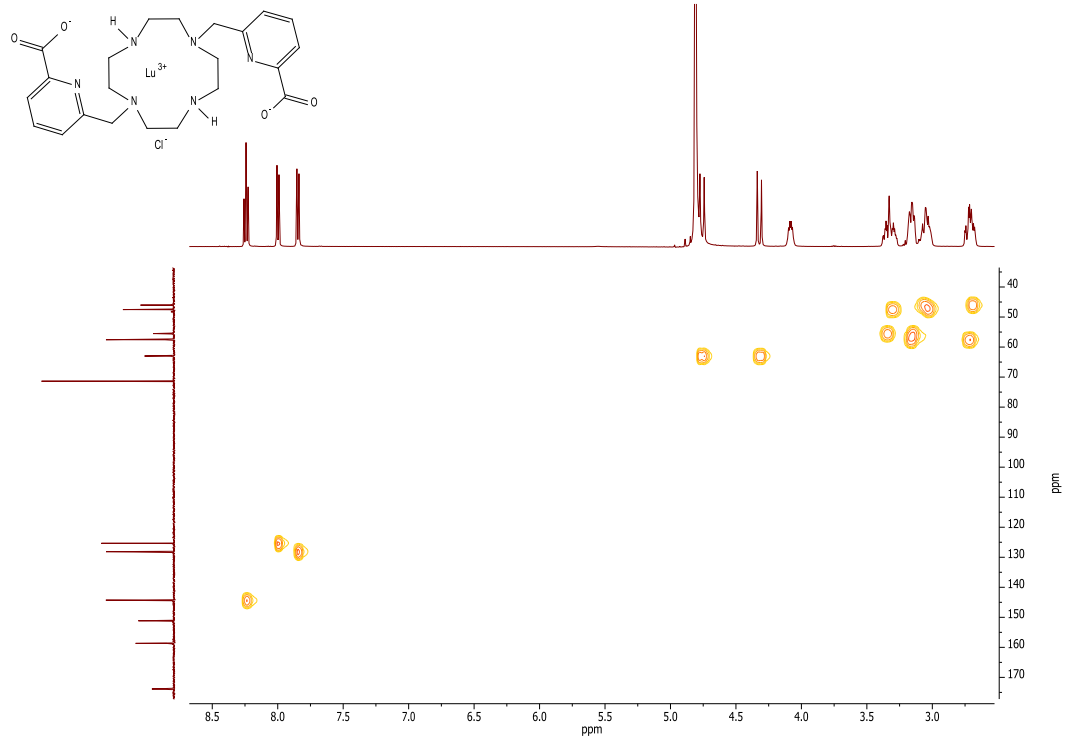
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



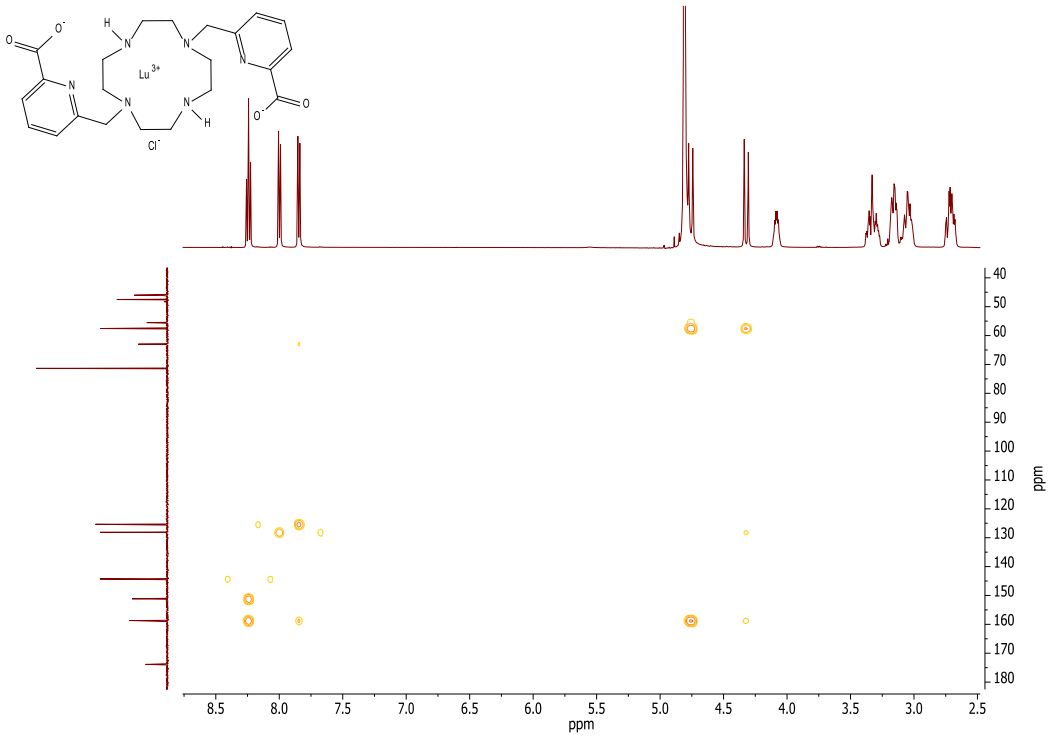
COSY-RMN (D_2O) (δ/ppm)



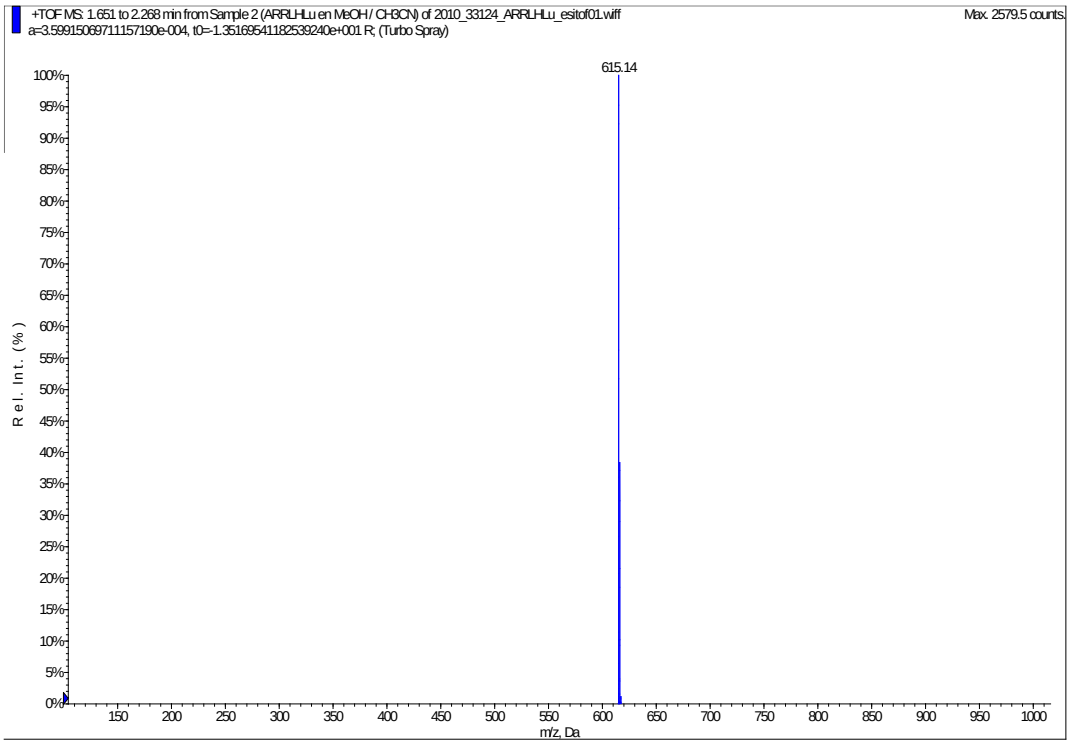
HSQC-RMN (D_2O) (δ/ppm)



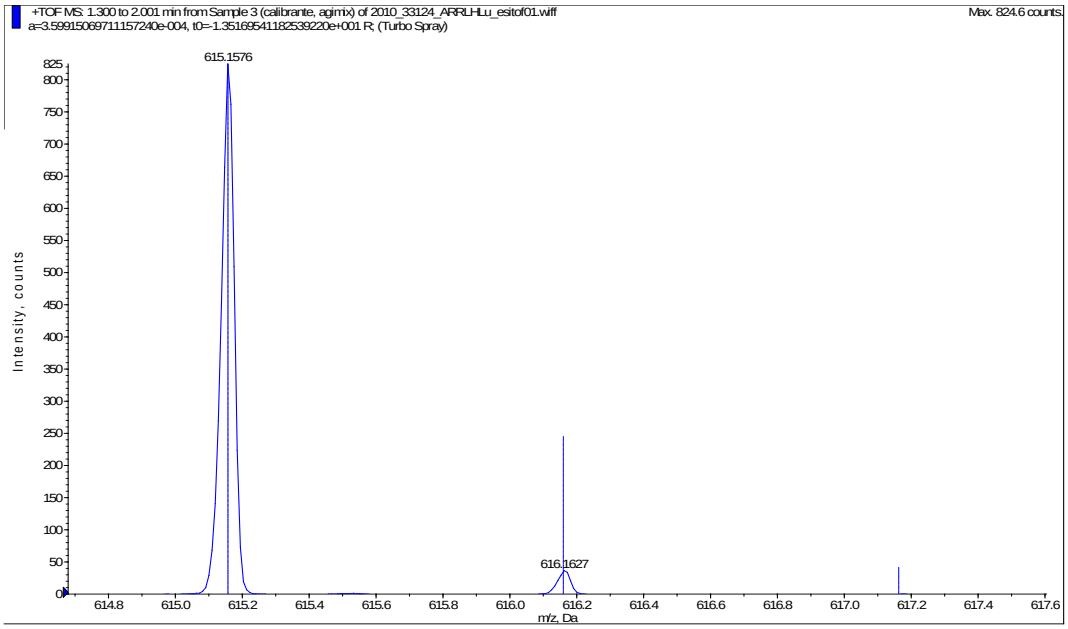
HMBC-RMN (D_2O) (δ/ppm)



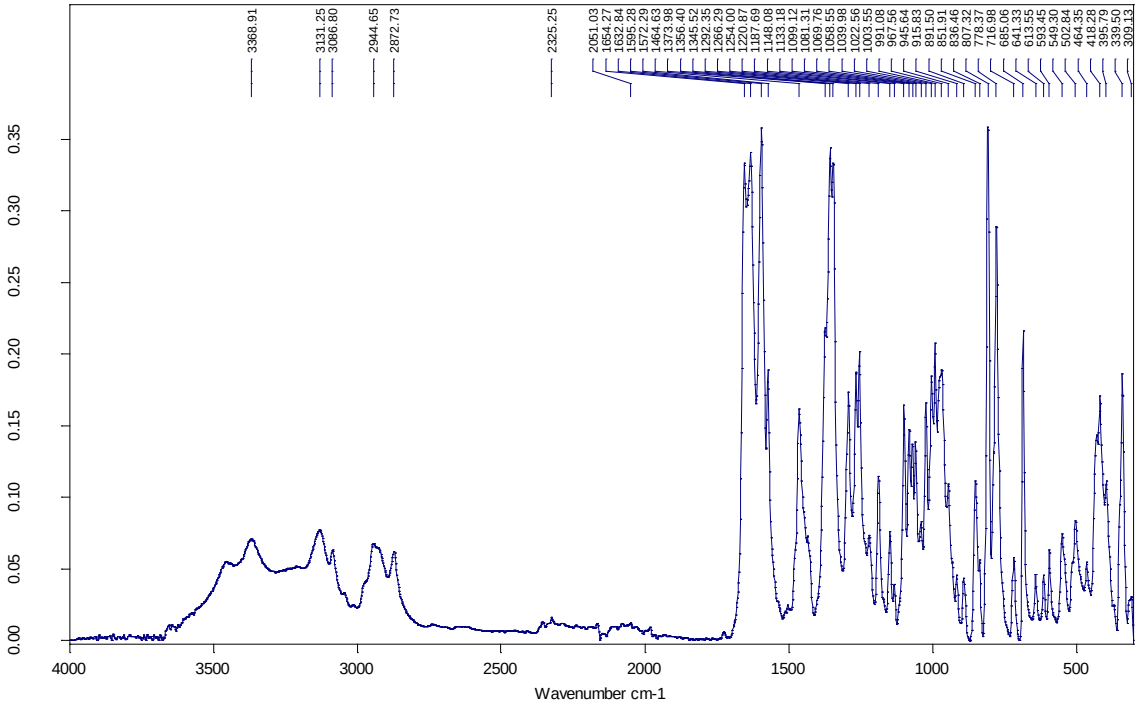
Espectro de masas ESI^+



Espectro ESI⁺ HR

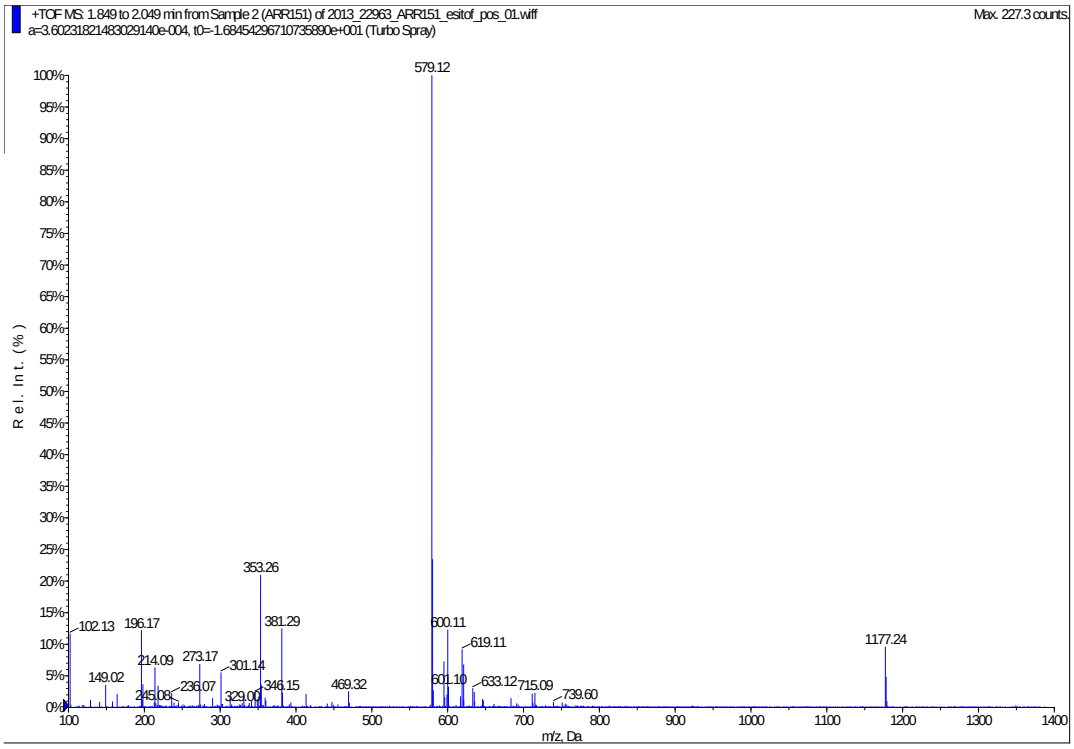


Espectro IR

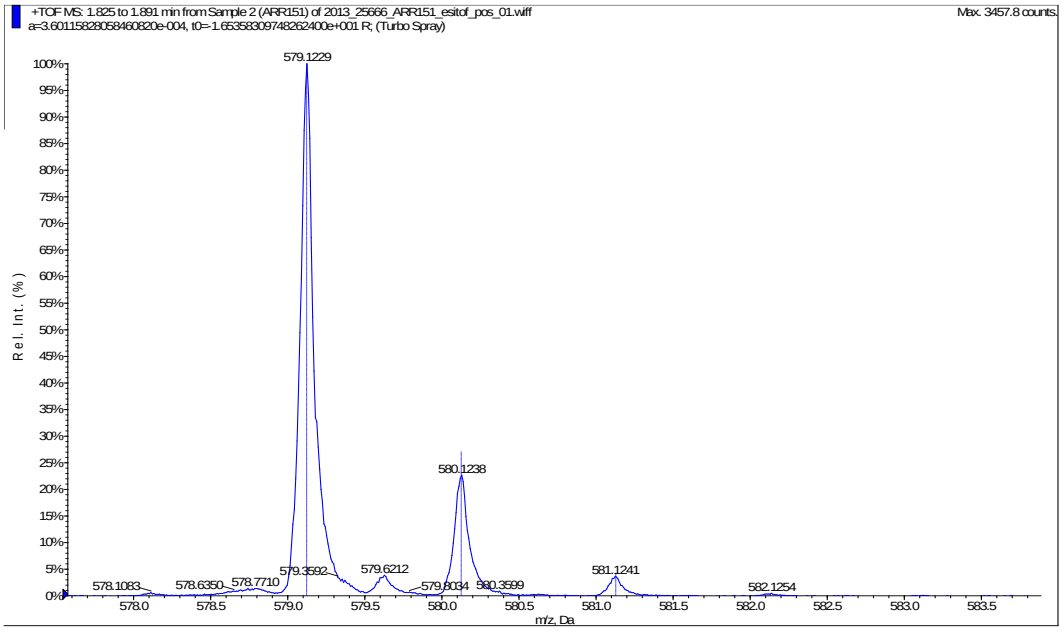


[La(dodpa)]OTf

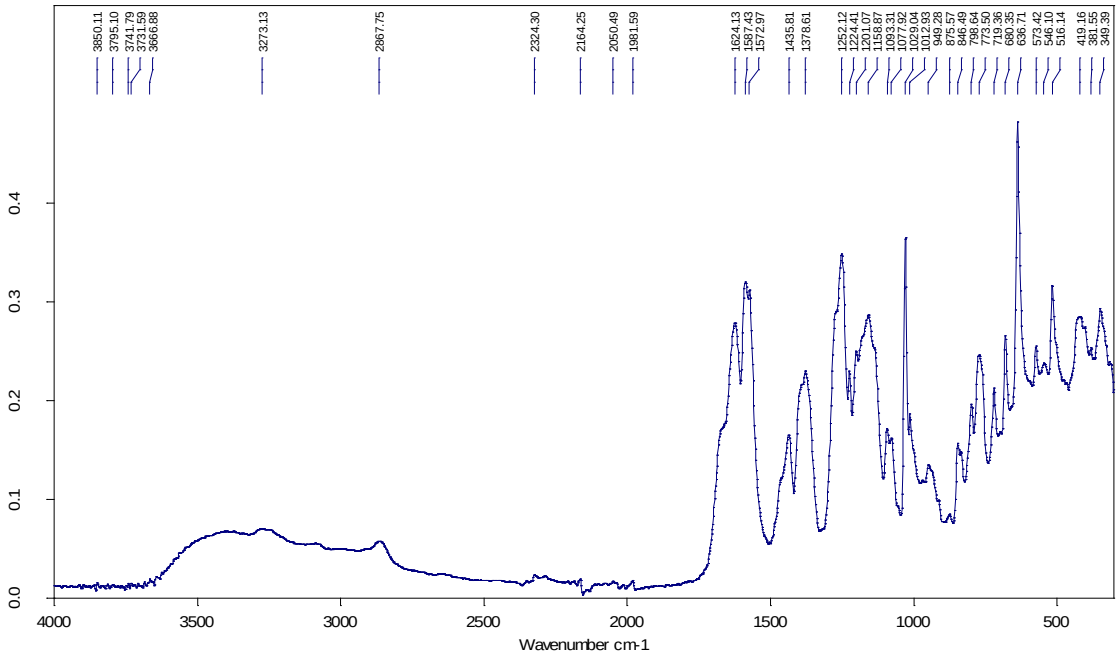
Espectro de masas ESI+



Espectro ESI+ HR

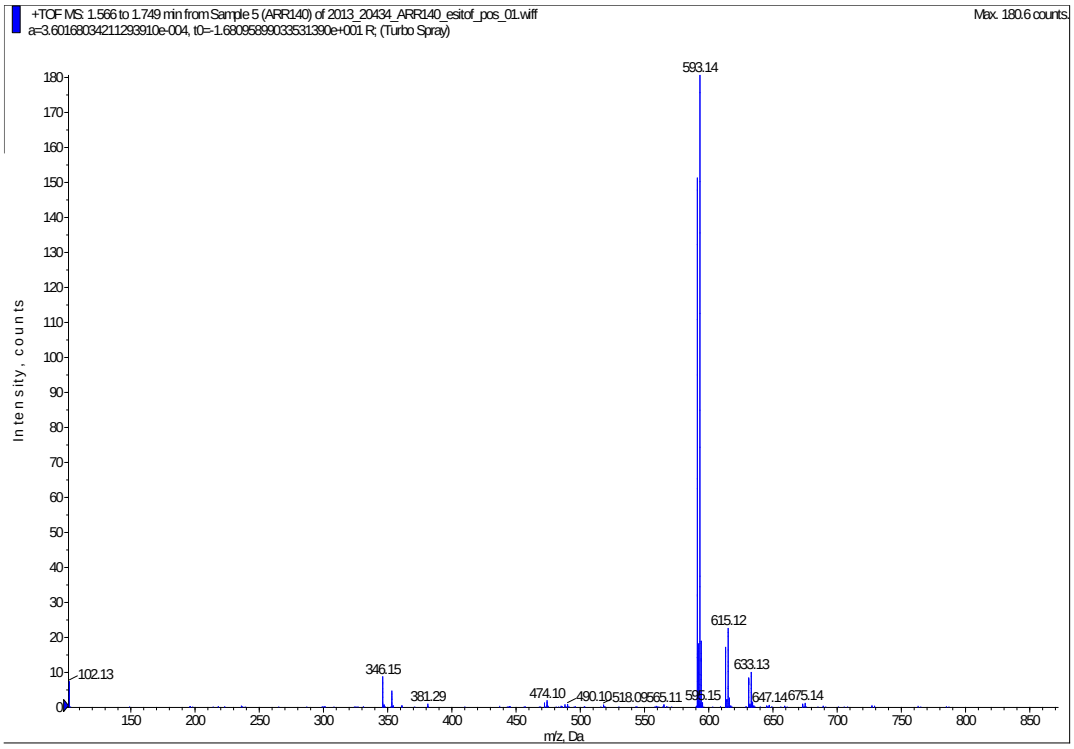


Espectro IR

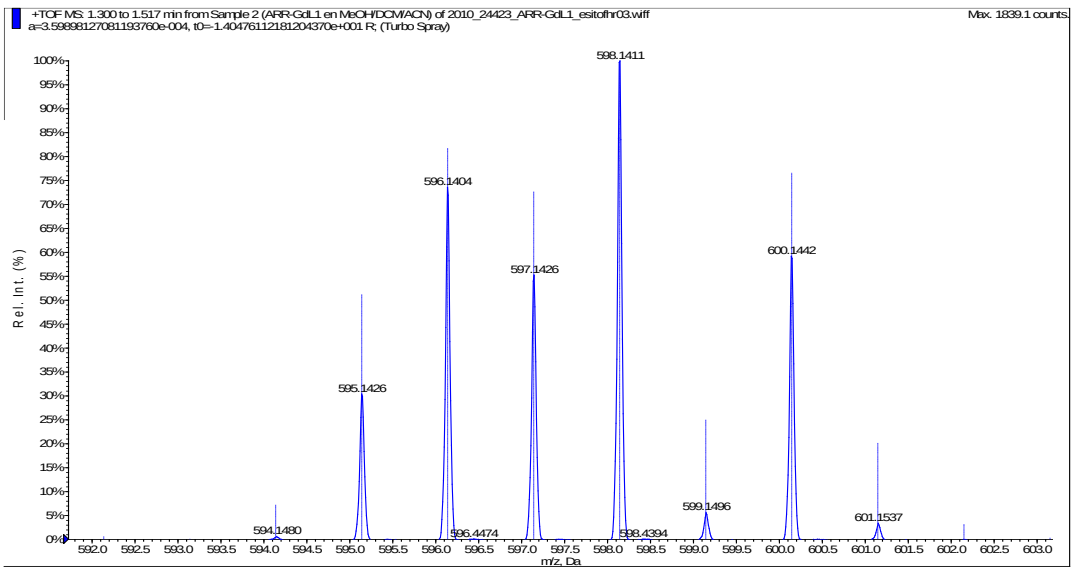

3850.11
3795.10
3741.79
3731.59
3666.88
3273.13
2867.75
2324.30
2164.25
2050.49
1981.59
1624.13
1587.43
1572.97
1435.81
1378.61
1252.12
1224.41
1201.07
1158.87
1093.31
1077.92
1023.94
1011.38
946.28
875.57
846.49
798.64
773.50
707.36
689.35
636.71
573.42
546.10
516.14
419.16
381.55
349.39
0.0
0.1
0.2
0.3
0.4
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Eu(dodpa)]OTf

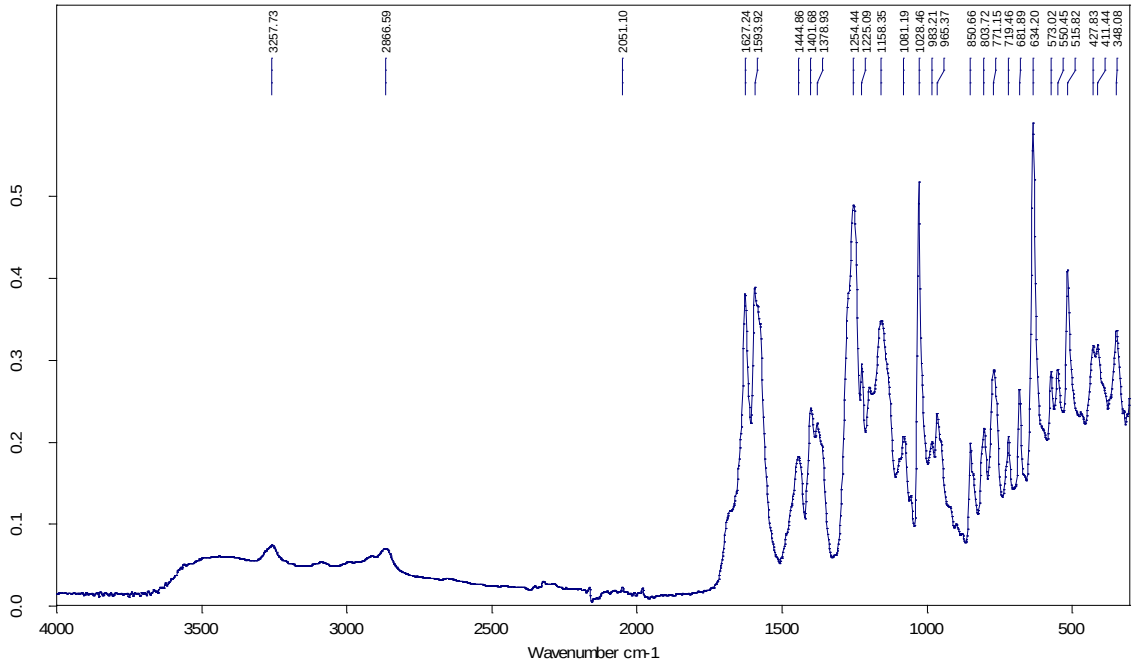
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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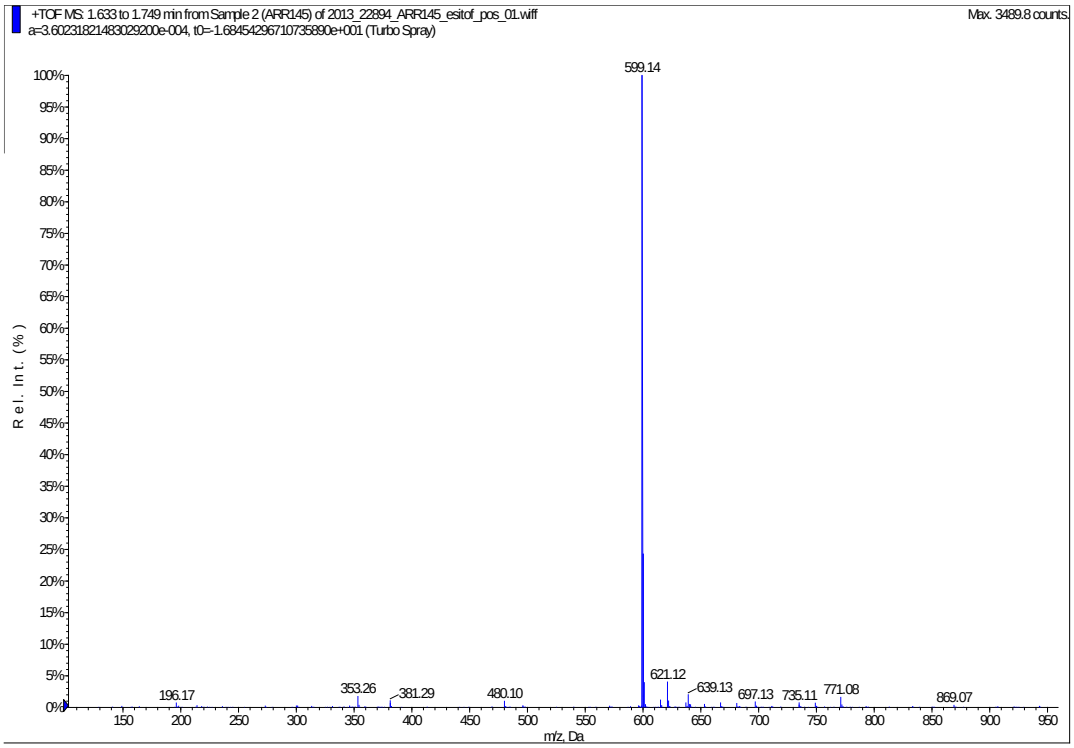
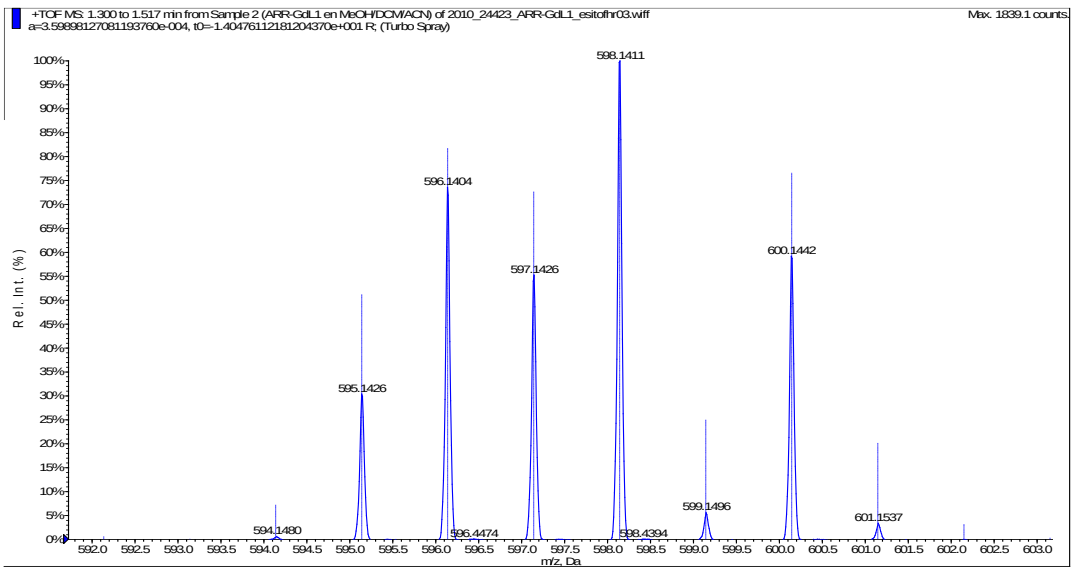
2051.10
1627.24
1593.92
1444.86
1401.68
1378.93
1254.44
1225.09
1158.35
1081.19
1028.46
983.21
965.37
850.66
803.72
771.15
719.46
681.89
634.20
573.02
550.45
515.82
427.83
411.44
348.08
0.0
0.1
0.2
0.3
0.4
0.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(dodpa)]OTf

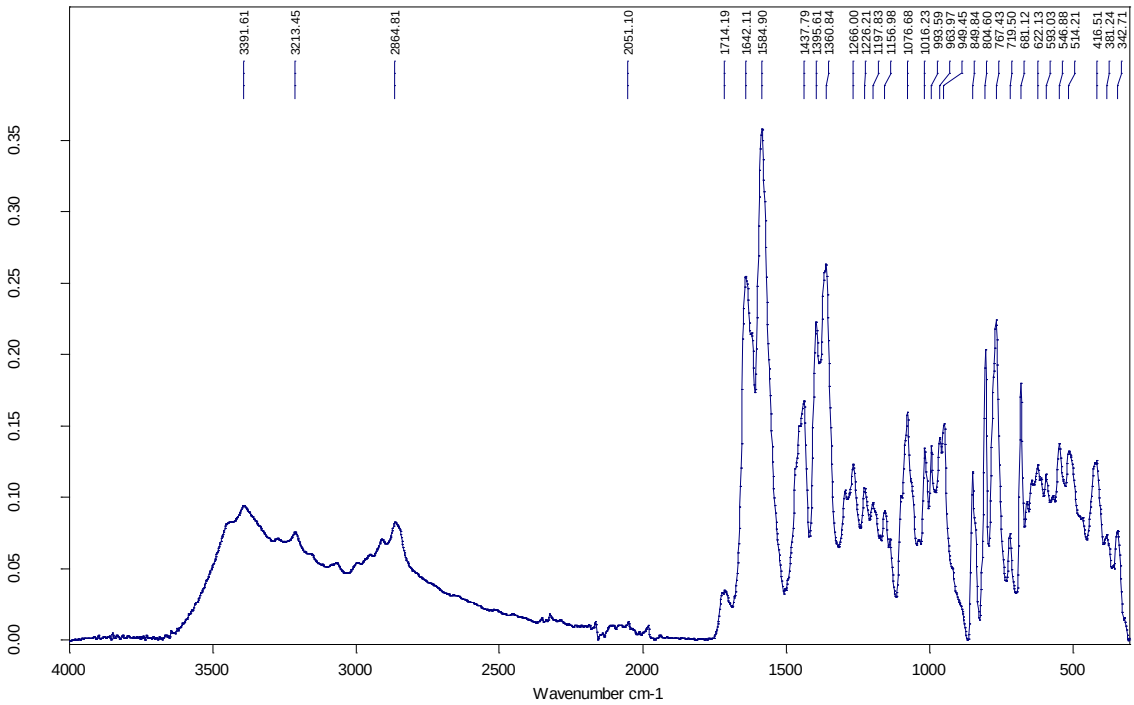
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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1360.84
1266.00
1226.21
1197.83
1156.98
1076.68
1016.23
993.59
967.07
949.45
849.84
804.60
767.43
719.50
681.12
622.13
593.03
546.88
514.21
416.51
381.24
342.71
0.00
0.05
0.10
0.15
0.20
0.25
0.30
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4000
3500
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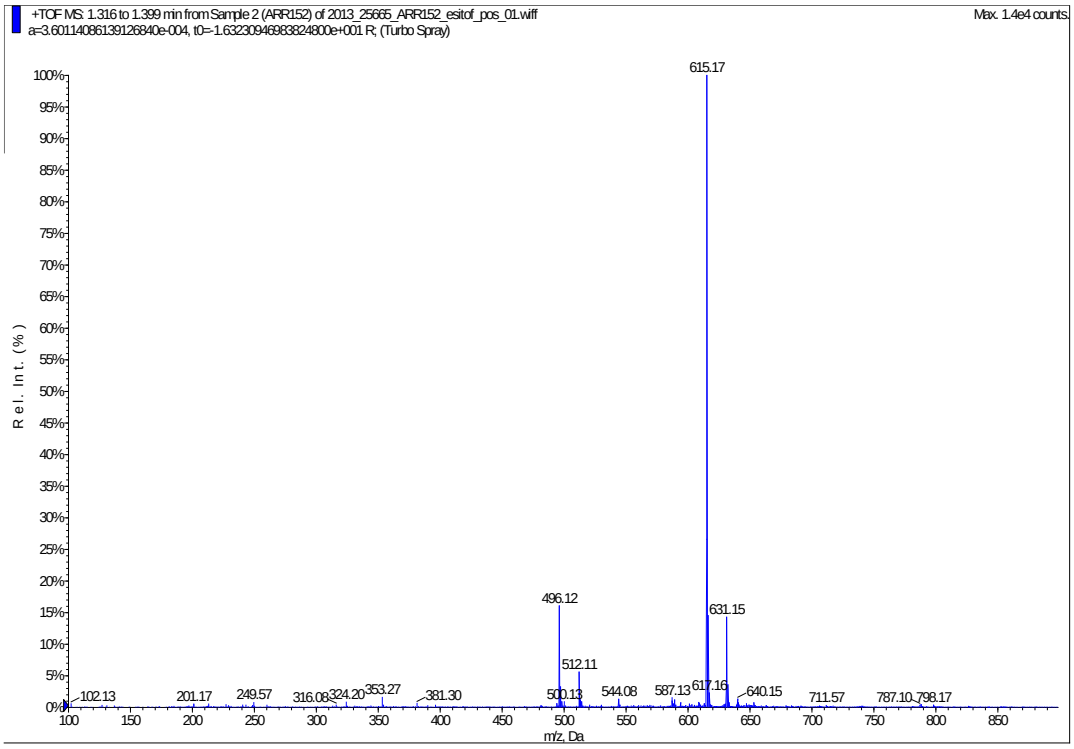
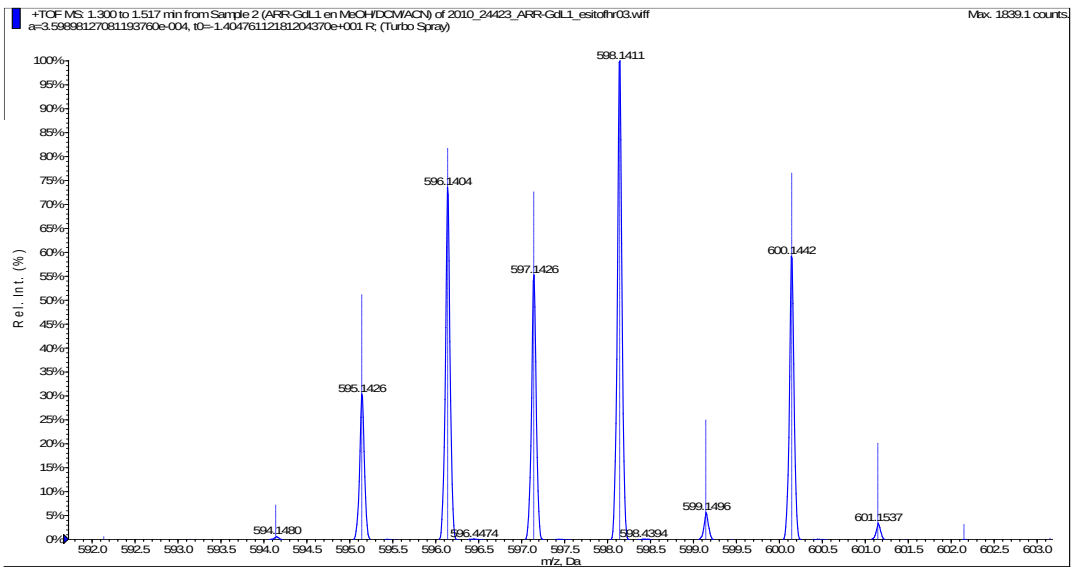
2500
2000
1500
1000
500
Wavenumber cm-1

[Lu(dodpa)]OTf

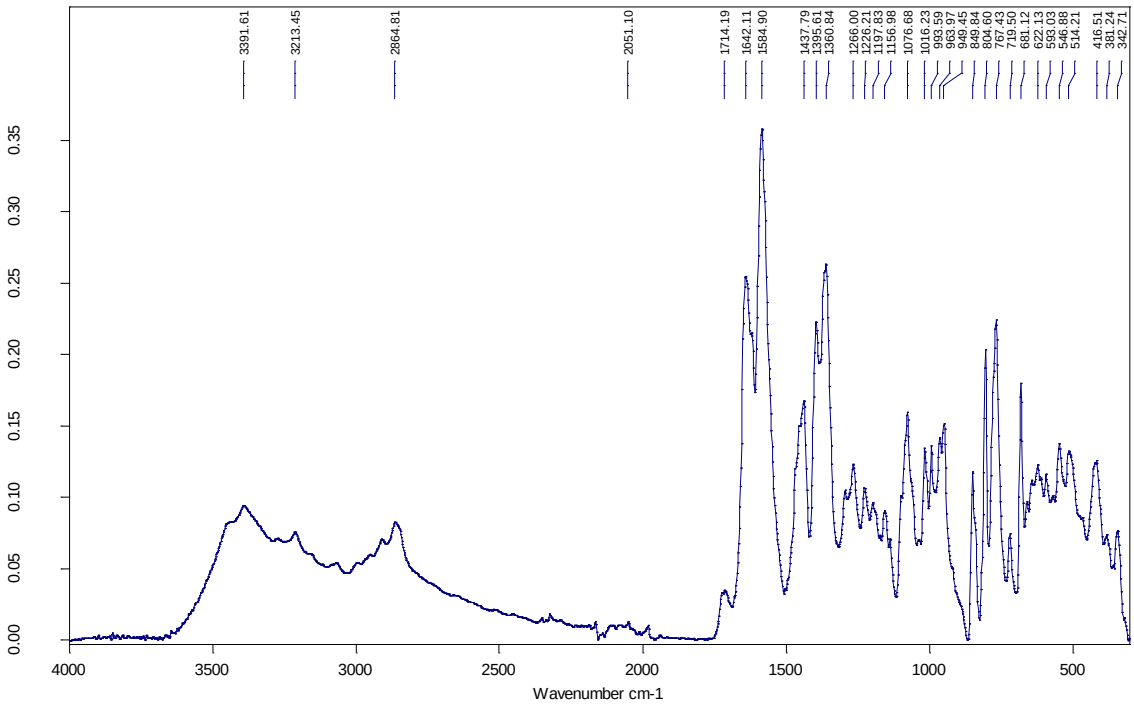
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR


3391.61
3213.45
2864.81
2051.10
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719.50
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622.13
593.03
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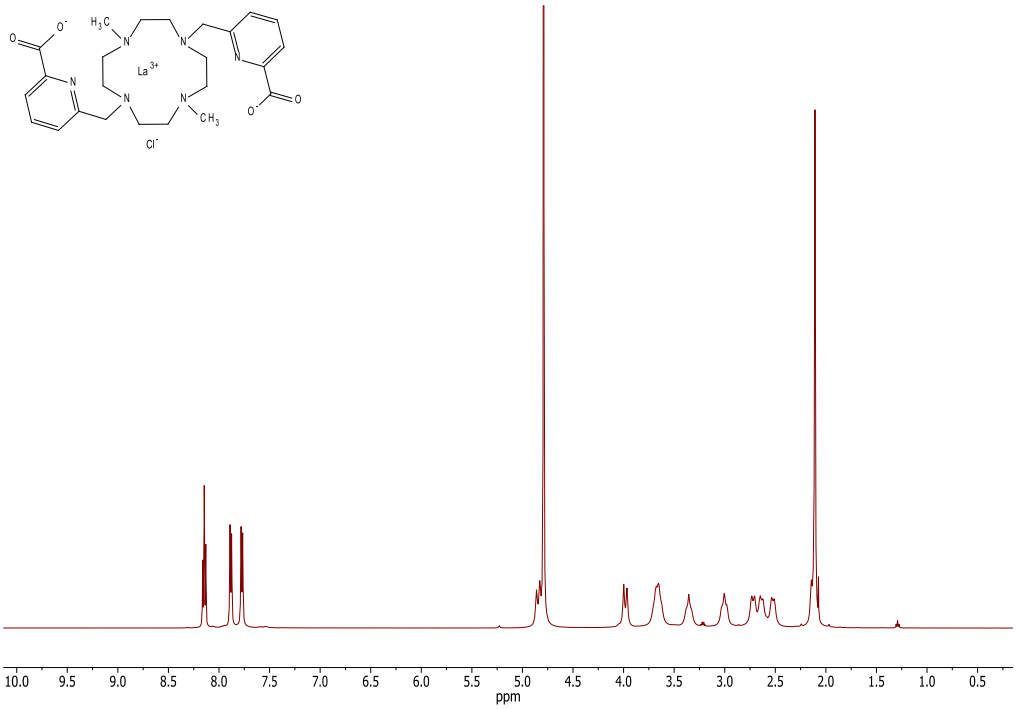
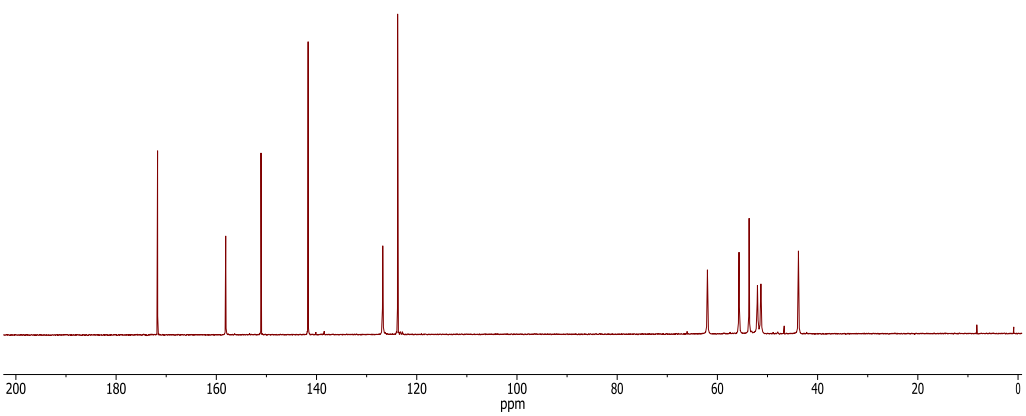
514.21
416.51
381.24
342.71
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[La(Me$_2$dodpa)]Cl

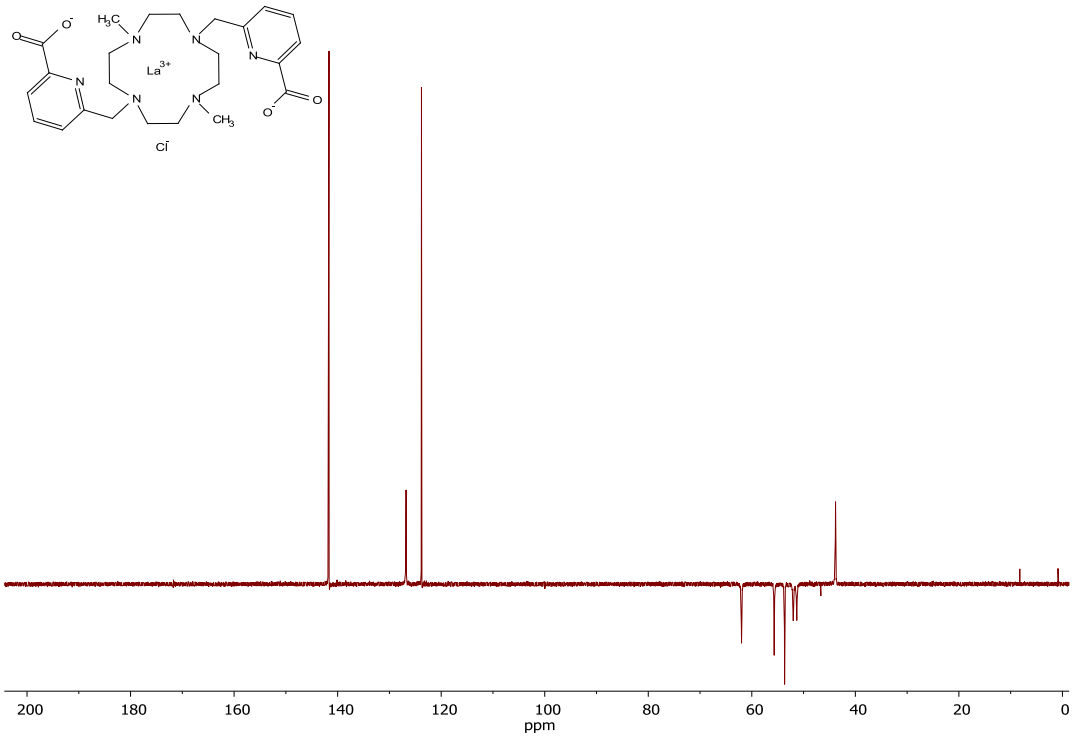
^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)



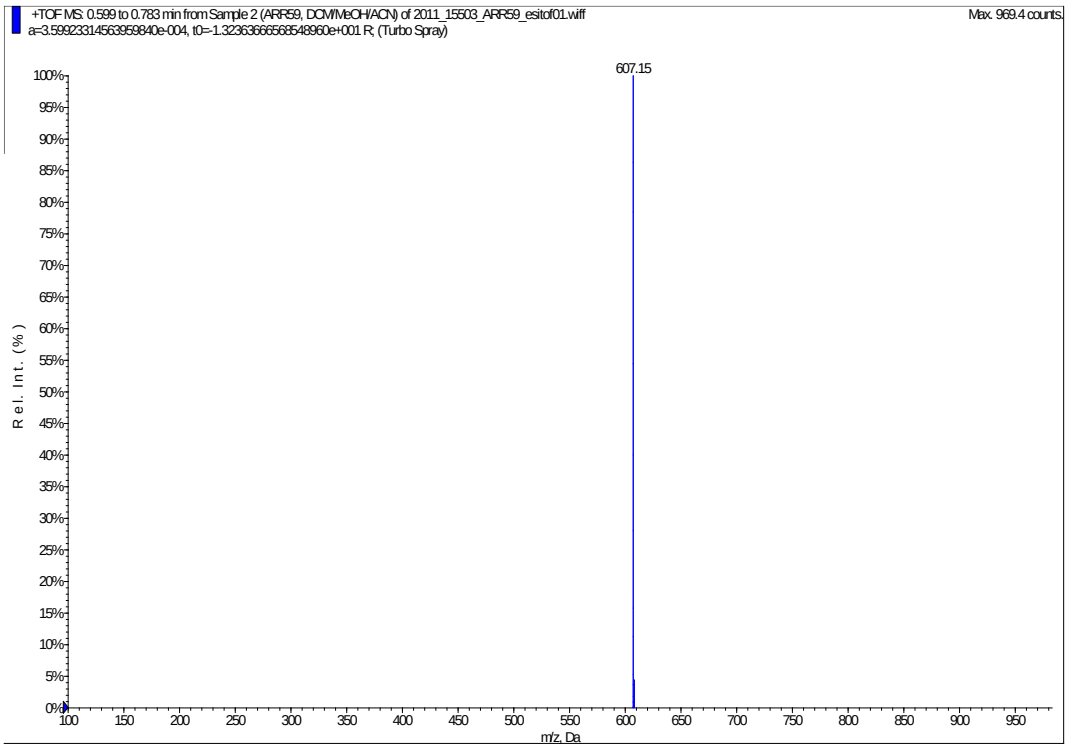
^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)



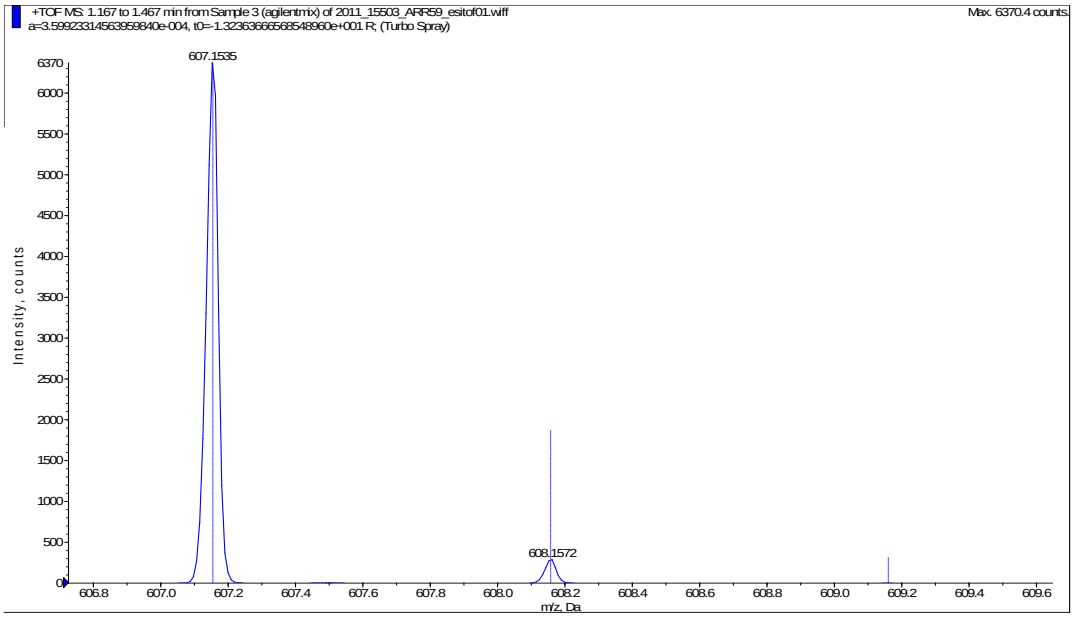
DEPT-RMN (D_2O) (δ/ppm)



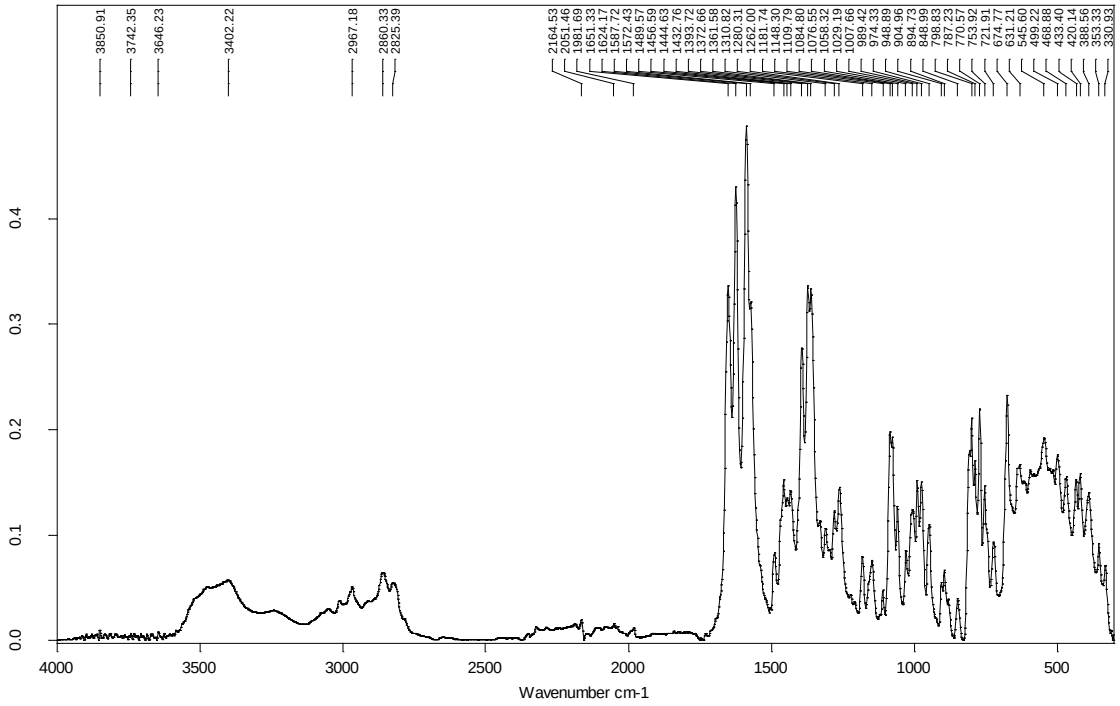
Espectro de masas ESI^+



Espectro ESI⁺ HR

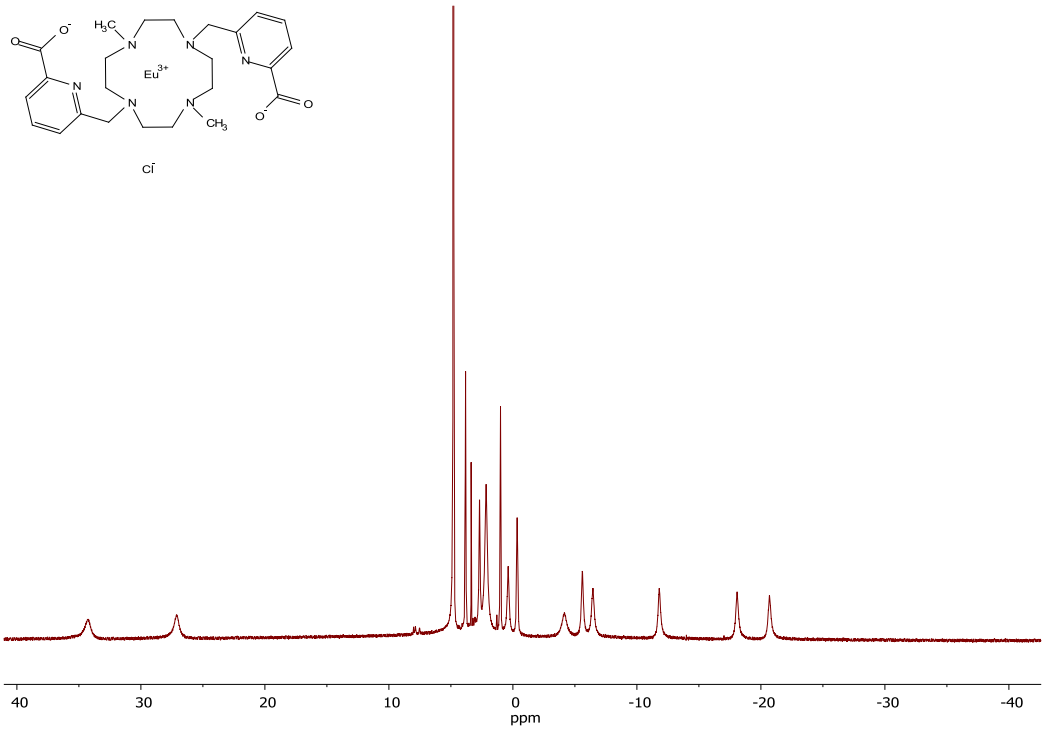


Espectro IR

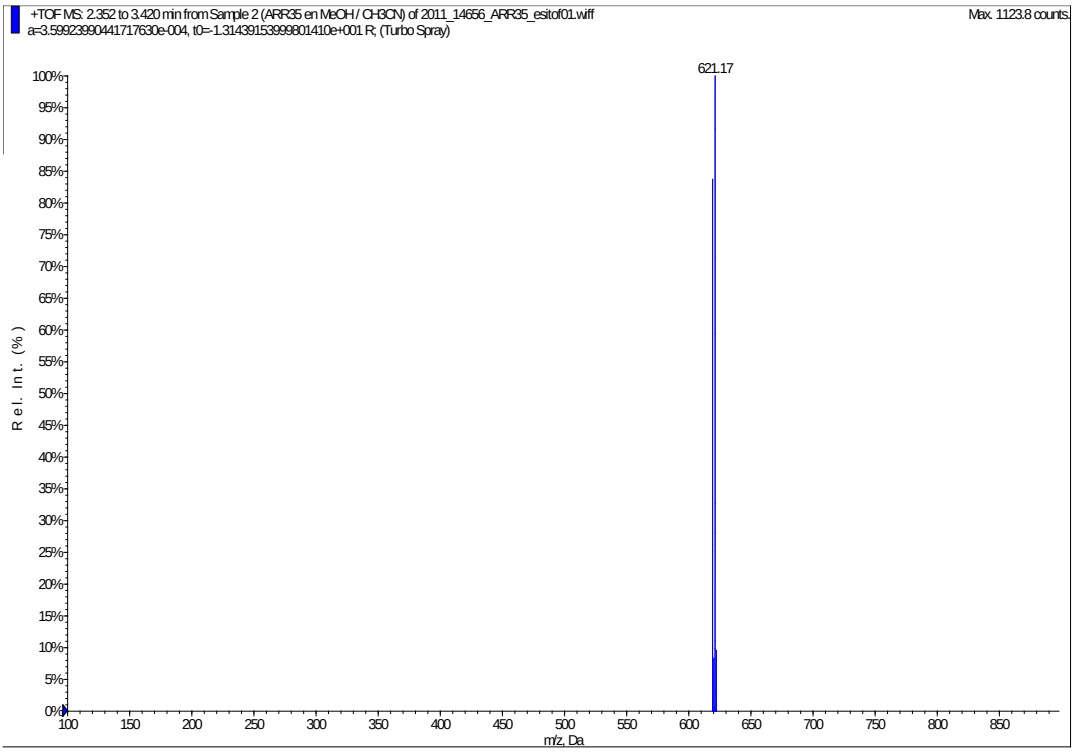


[Eu(Me$_2$dodpa)]Cl

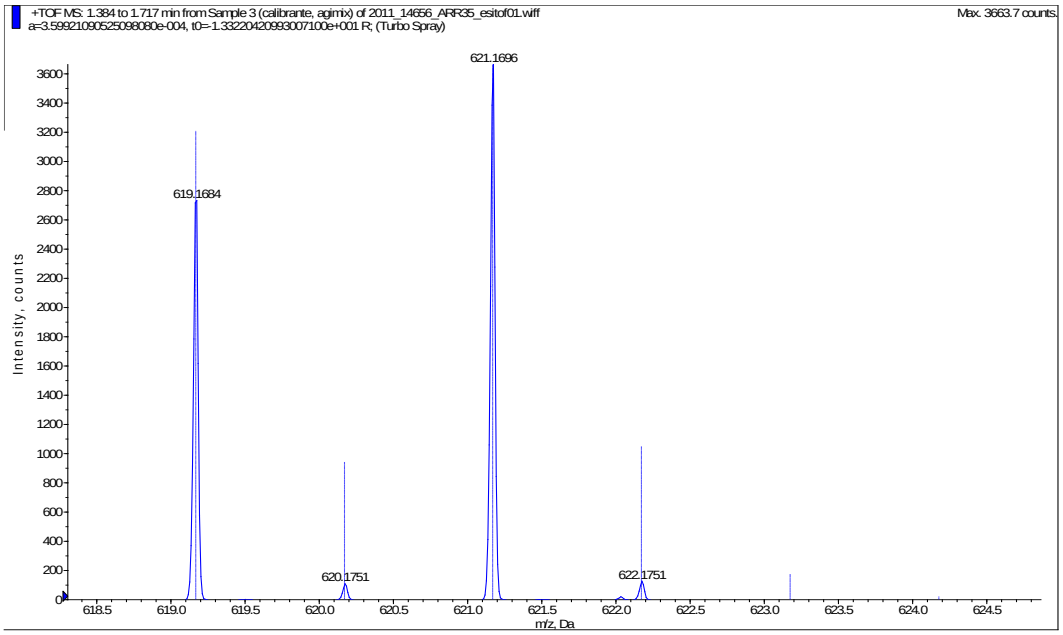
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



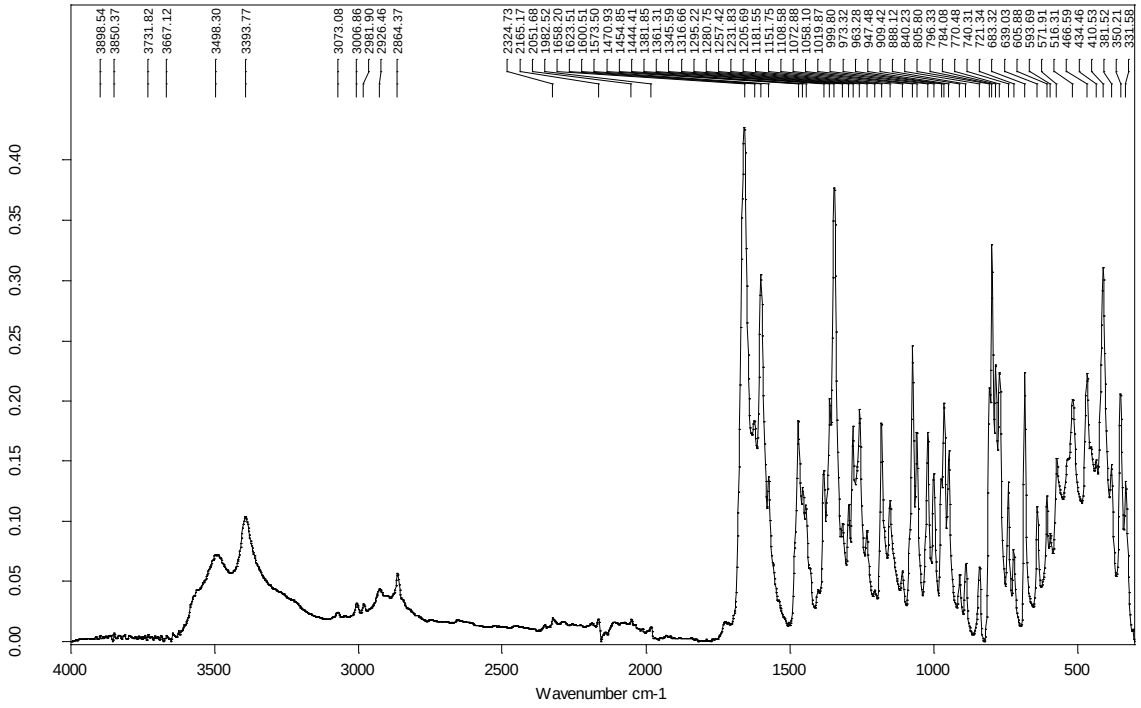
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

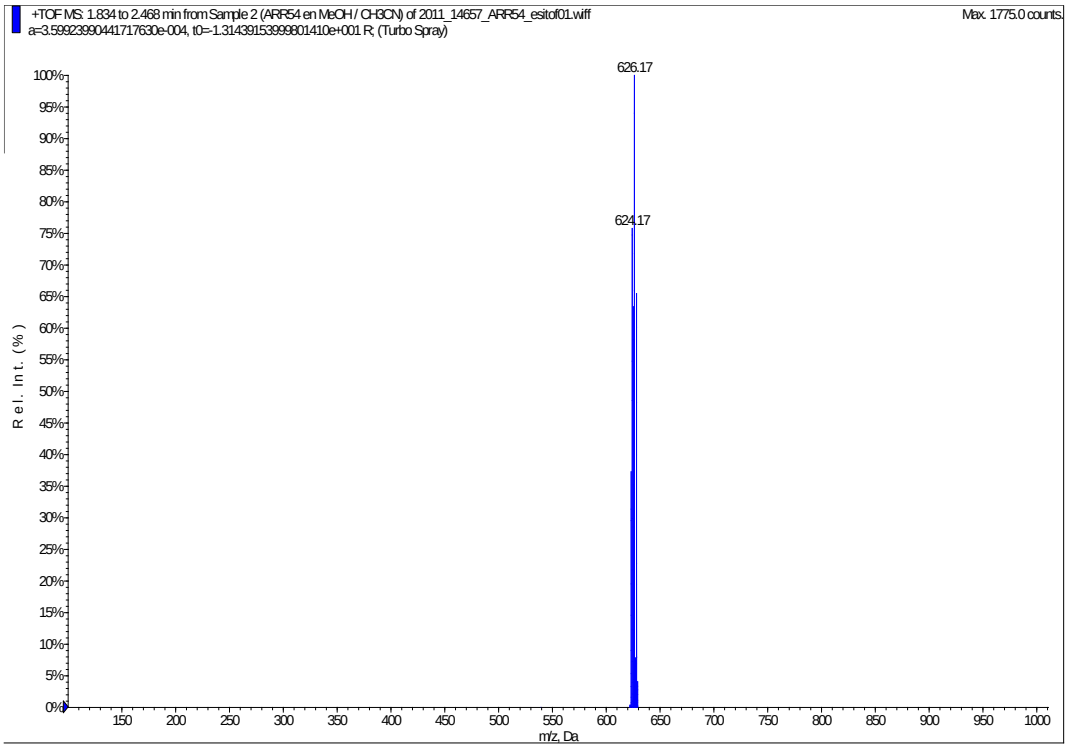


Espectro IR

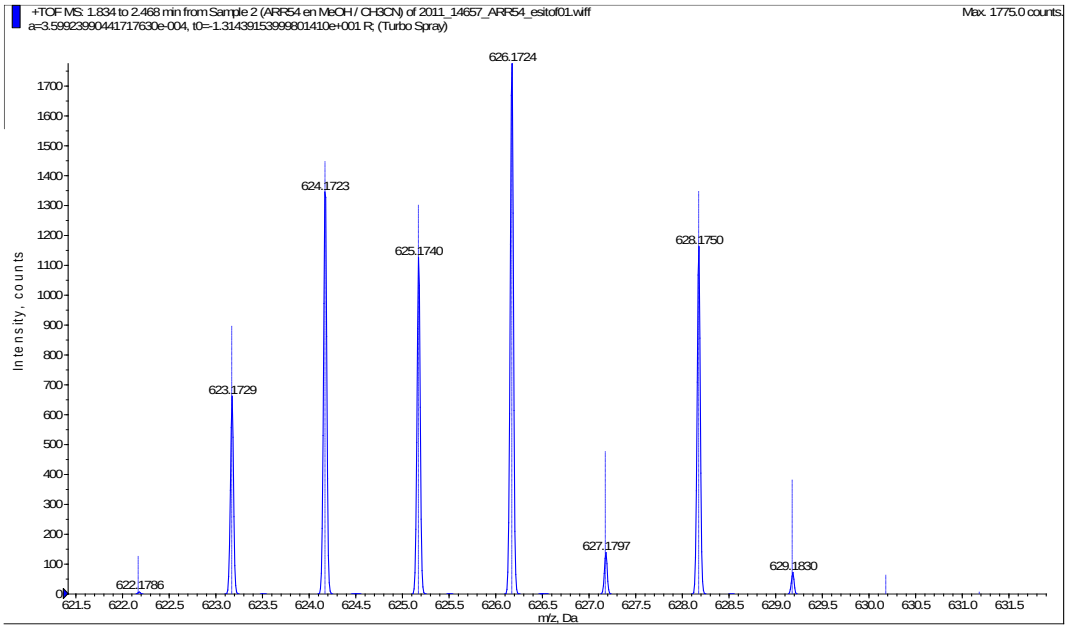


[Gd(Me$_2$dodpa)]Cl

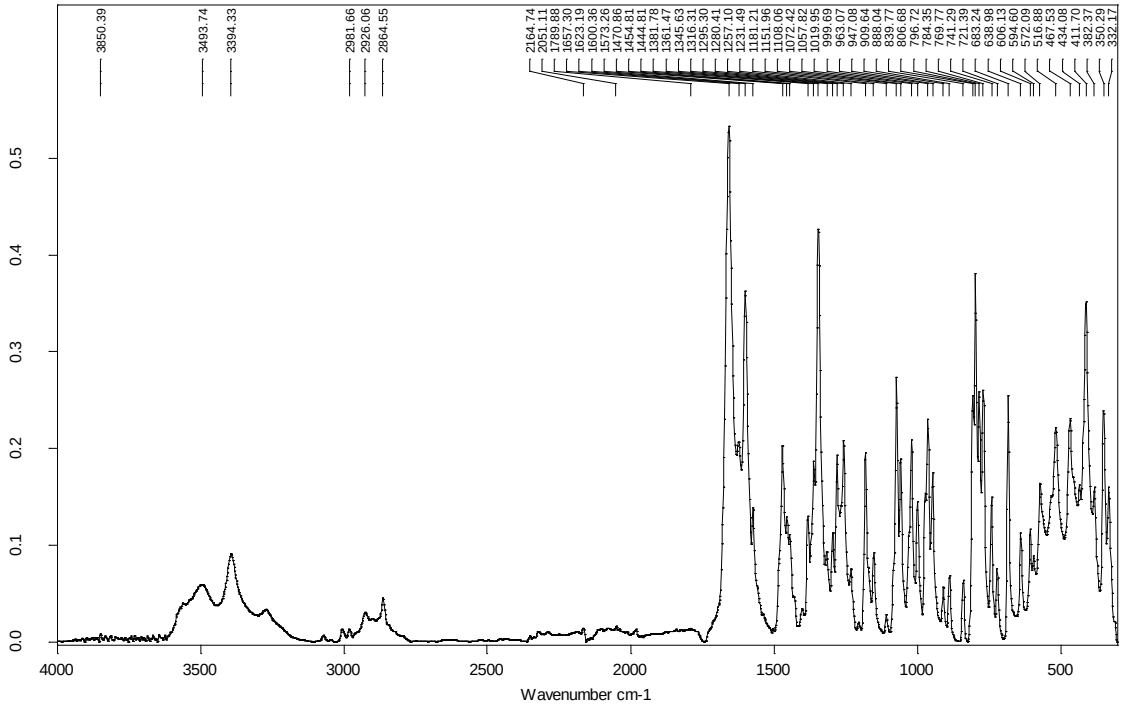
Espectro de masas ESI$^+$



Espectro ESI$^+$ HR



Espectro IR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2981.66
2926.06
2864.55
2164.74
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1789.88
1657.30
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1600.36
1573.26
1470.86
1454.81
1444.81
1381.78
1361.47
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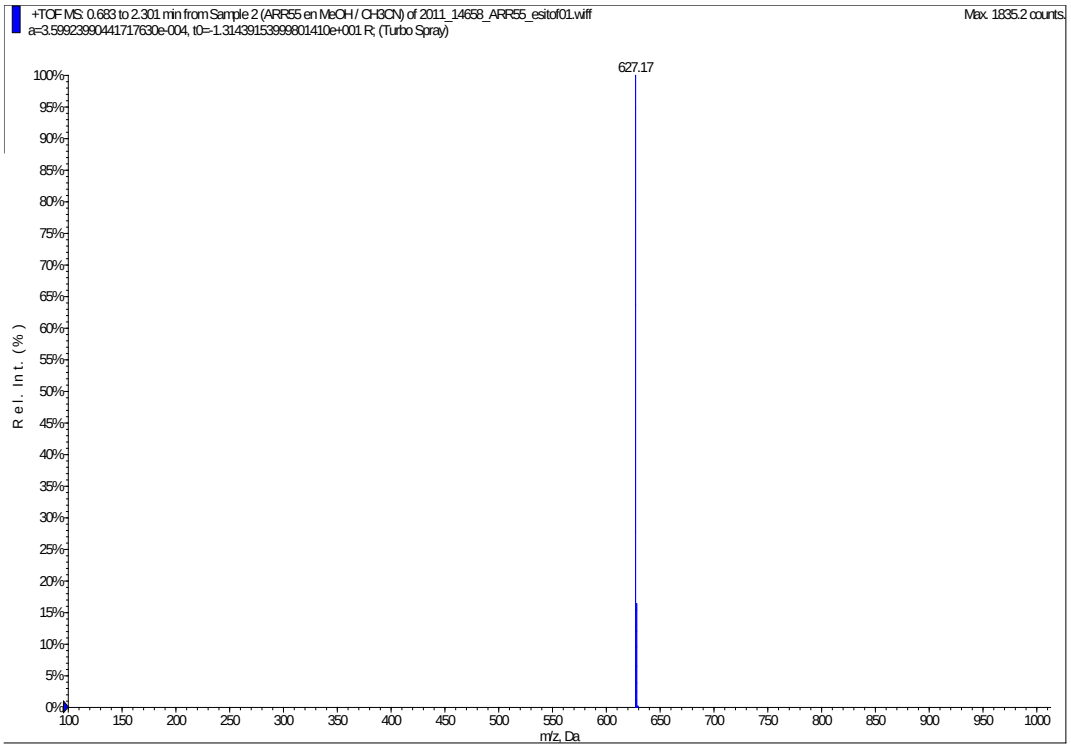
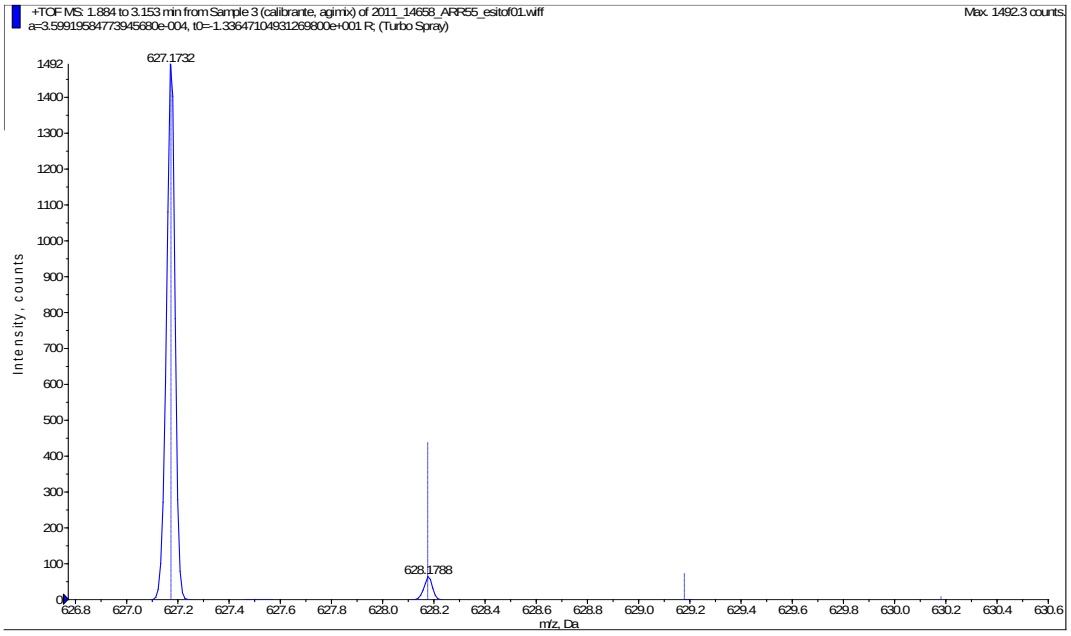
1316.31
1295.30
1280.41
1257.10
1231.49
1181.21
1151.96
1108.06
1072.42
1057.82
1019.95
999.69
963.07
947.08
909.64
888.04
839.77
806.68
796.72
784.35
769.77
741.39
721.39
683.24
638.98
606.13
594.60
572.09
516.88
467.53
434.08
414.70
382.37
350.29
332.17
0.0
0.1
0.2
0.3
0.4
0.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(Me$_2$dodpa)]Cl

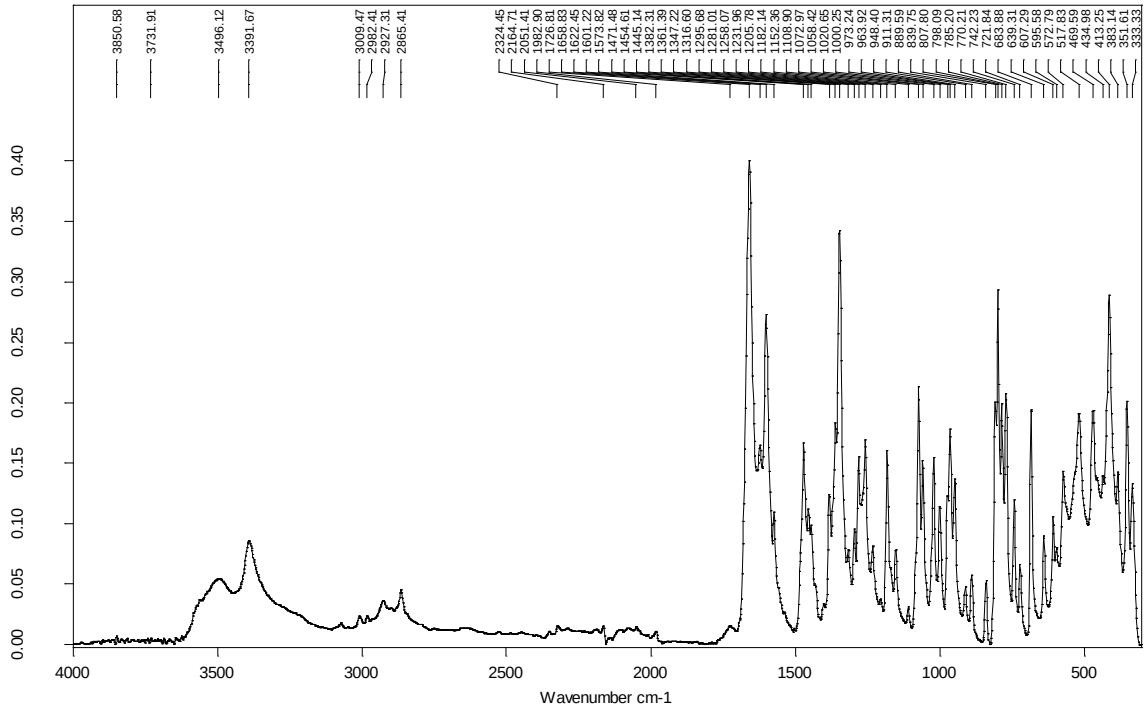
Espectro de masas ESI$^+$



Espectro ESI$^+$ HR



Espectro IR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3496.12
3391.67
3009.47
2982.41
2927.31
2865.41
2324.45
2164.71
2051.41
1982.90
1728.81
1658.88
1622.45
1601.22
1573.82
1471.48
1454.61
1445.14
1382.31
1361.39
1347.27
1316.60
1295.68
1281.01
1258.07
1231.96
1205.78
1182.14
1152.36
1109.90
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1020.65
1000.25
973.24
963.92
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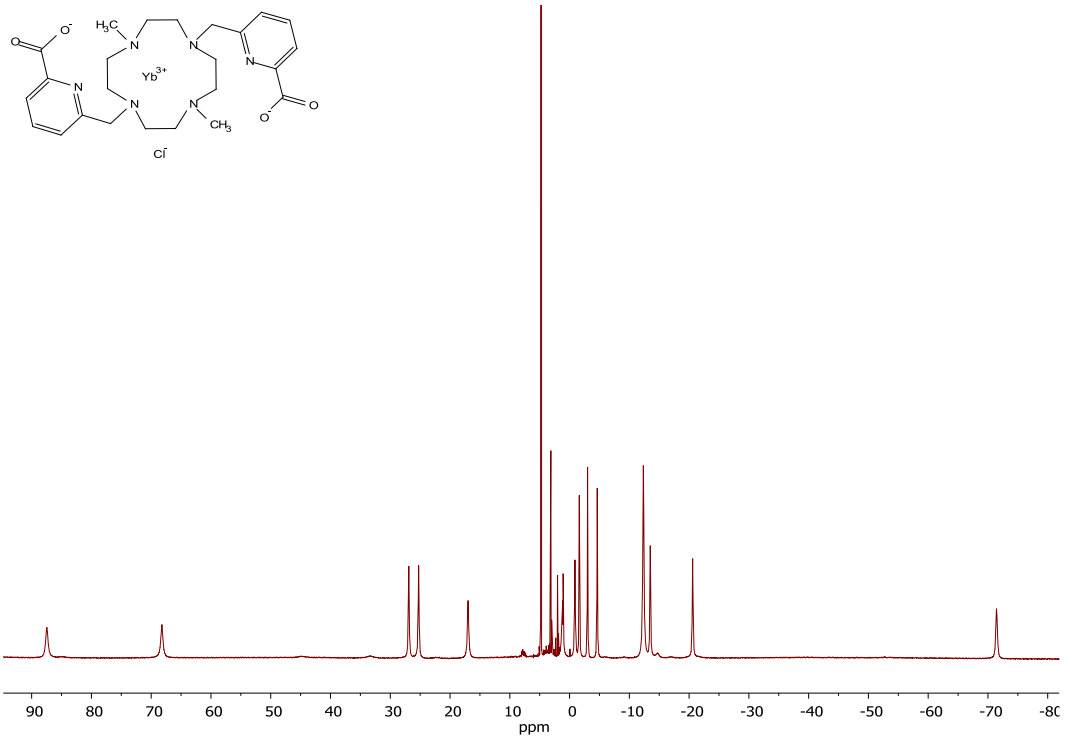
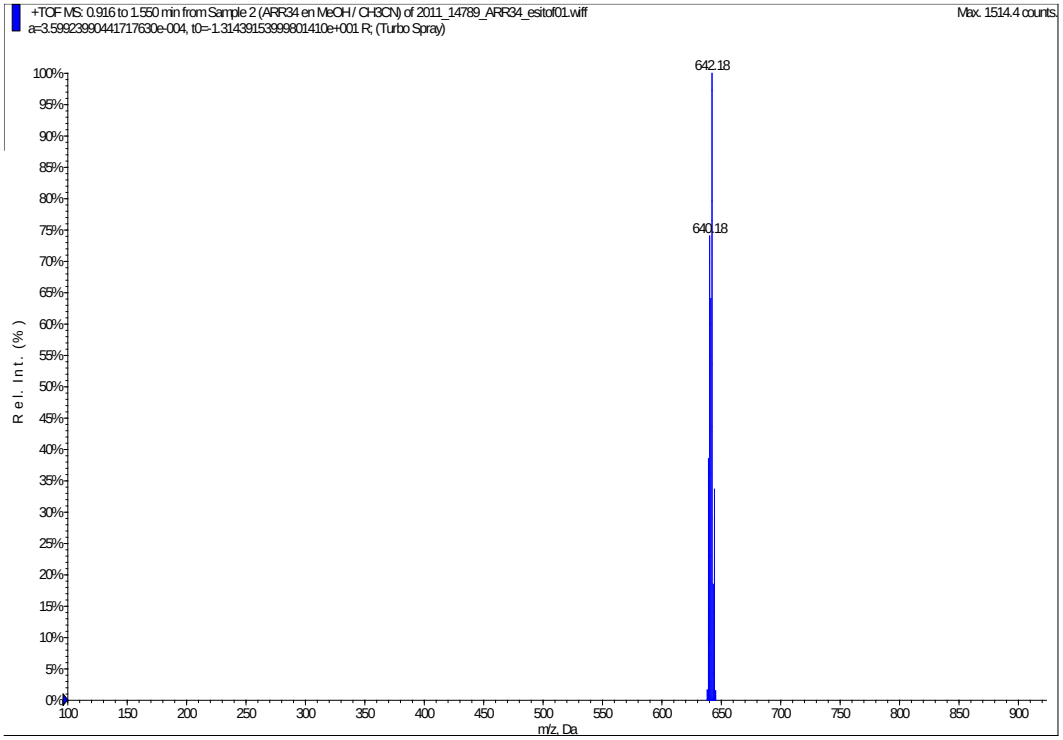
434.98
413.25
383.14
357.61
333.33
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Yb(Me$_2$dodpa)]Cl

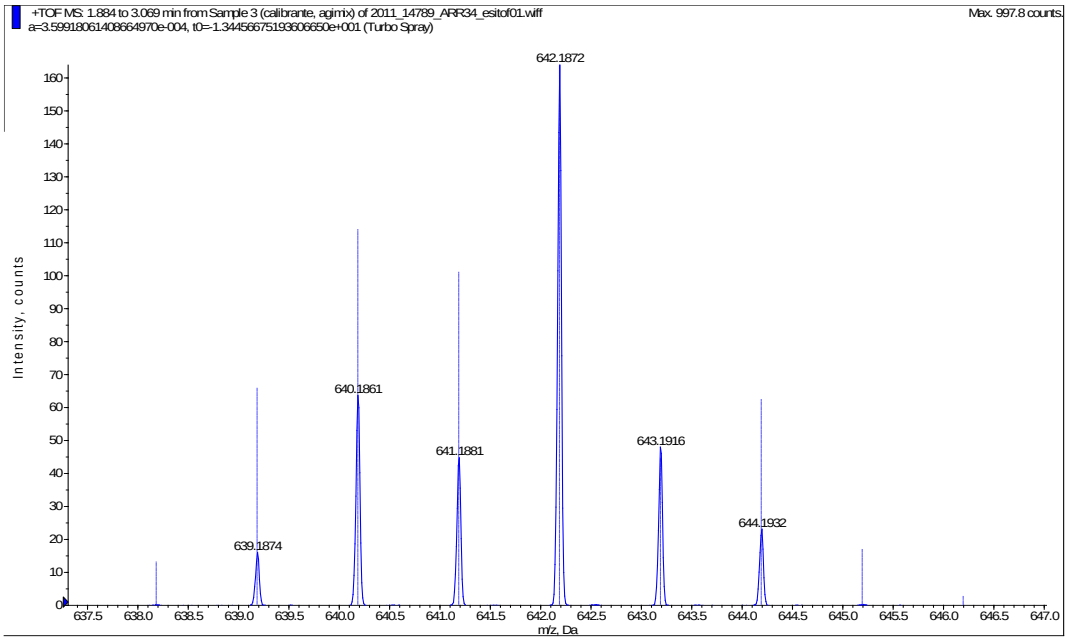
^{1}H-RMN (D_2O, 278K, 500 MHz) (δ/ppm)



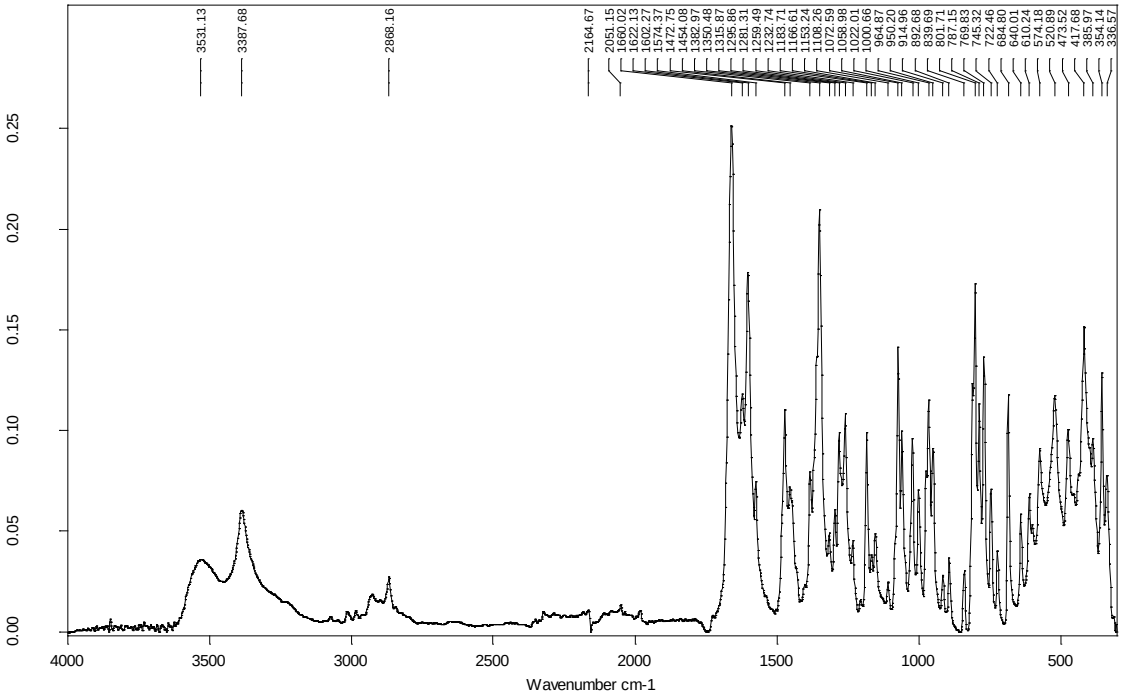
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

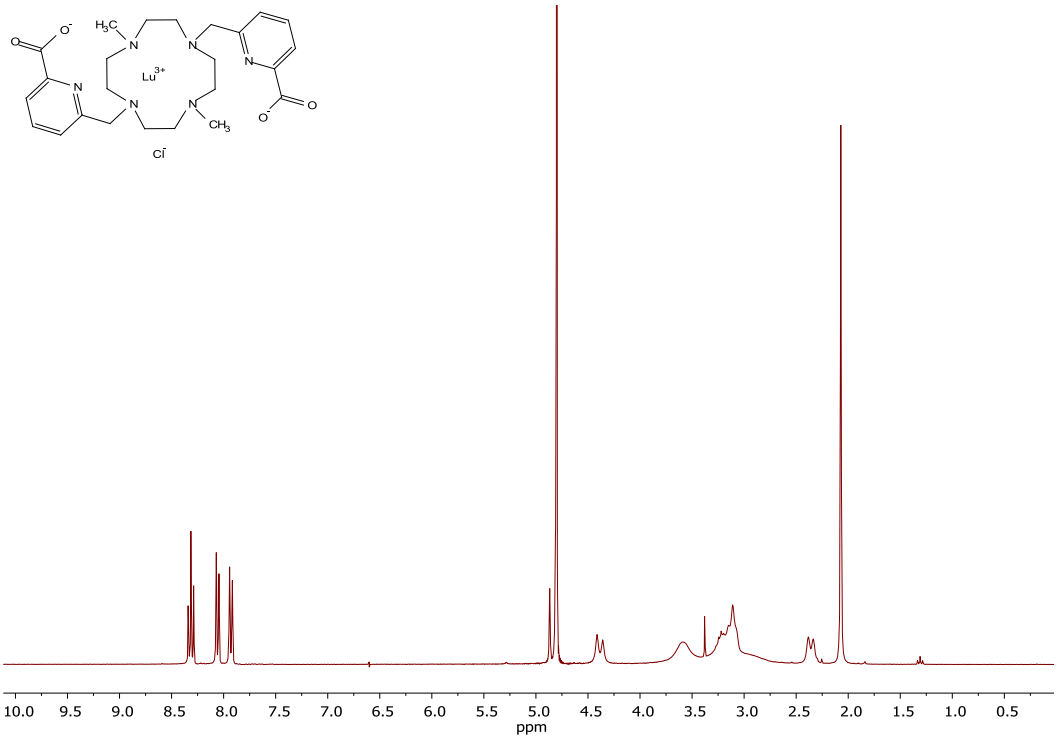


Espectro IR

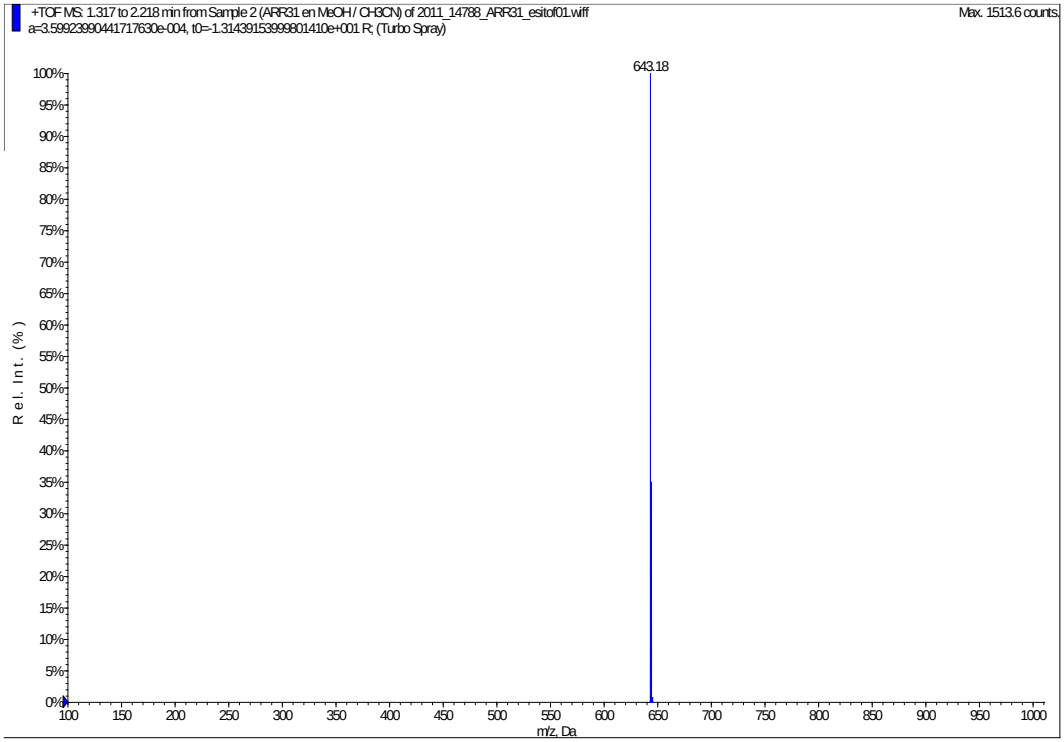


[Lu(Me$_2$dodpa)]Cl

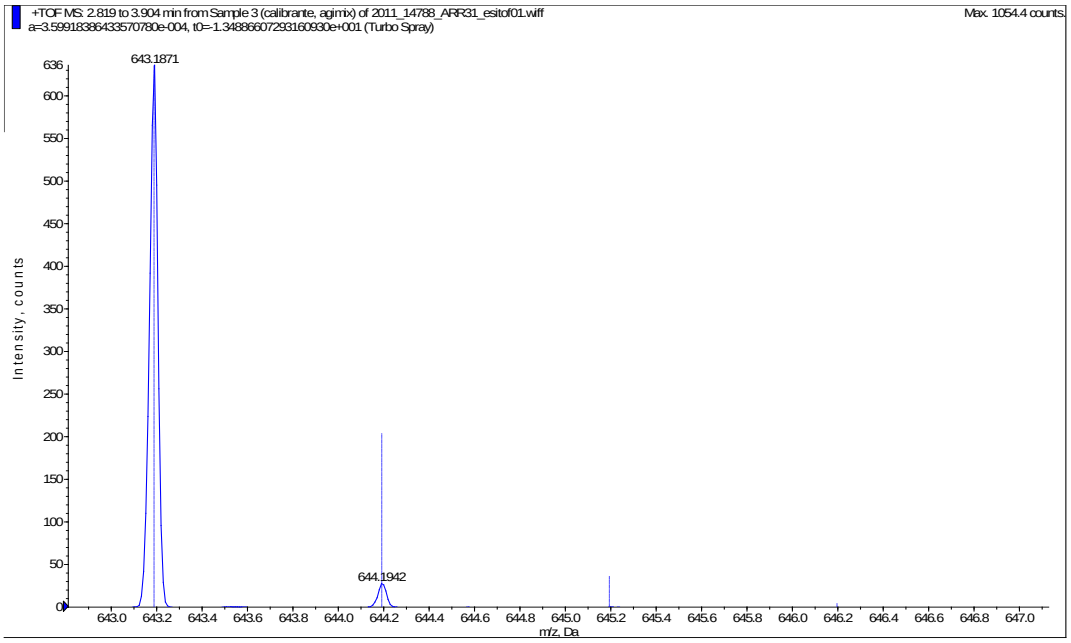
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



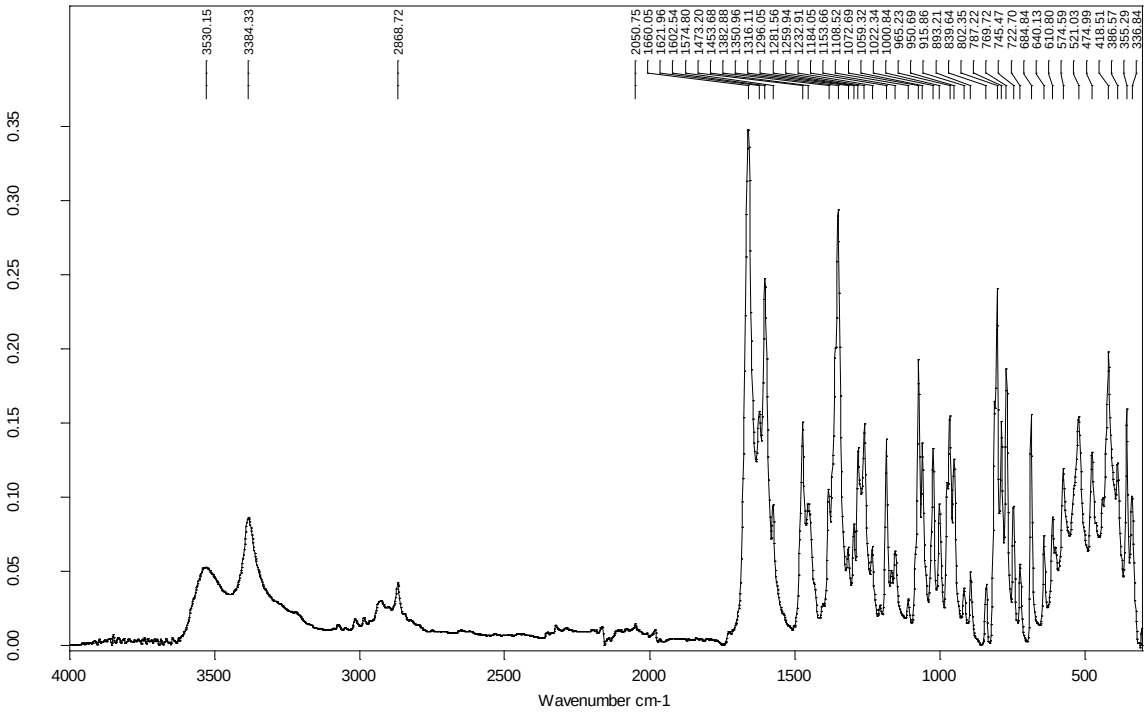
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

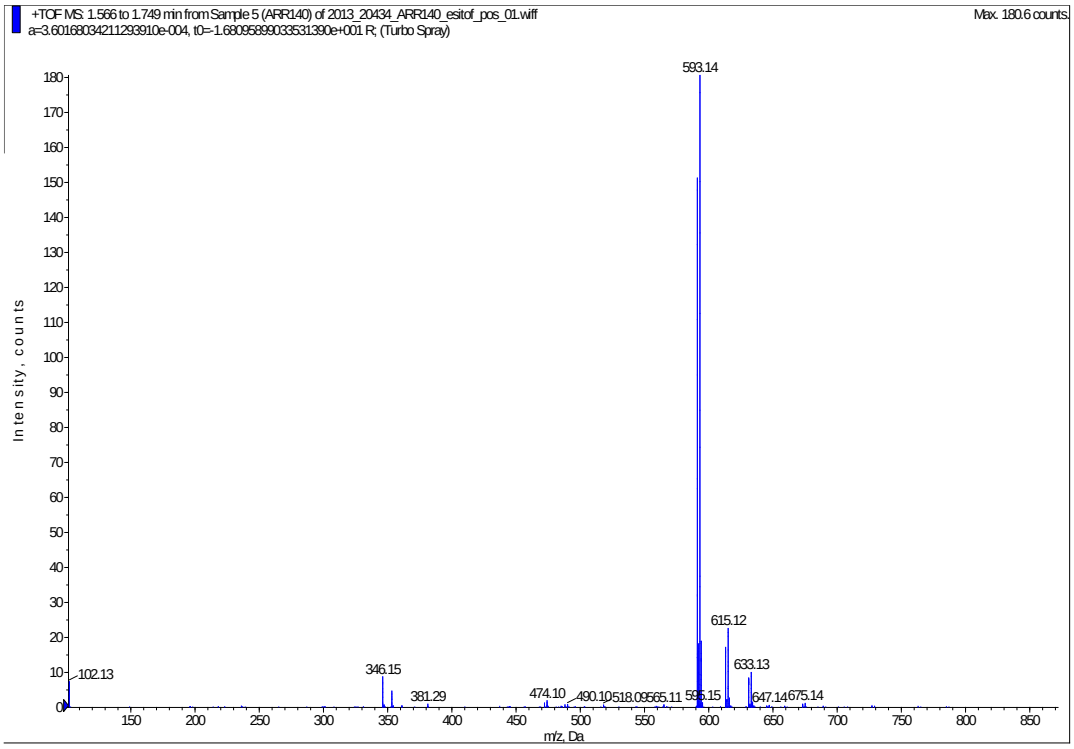


Espectro IR

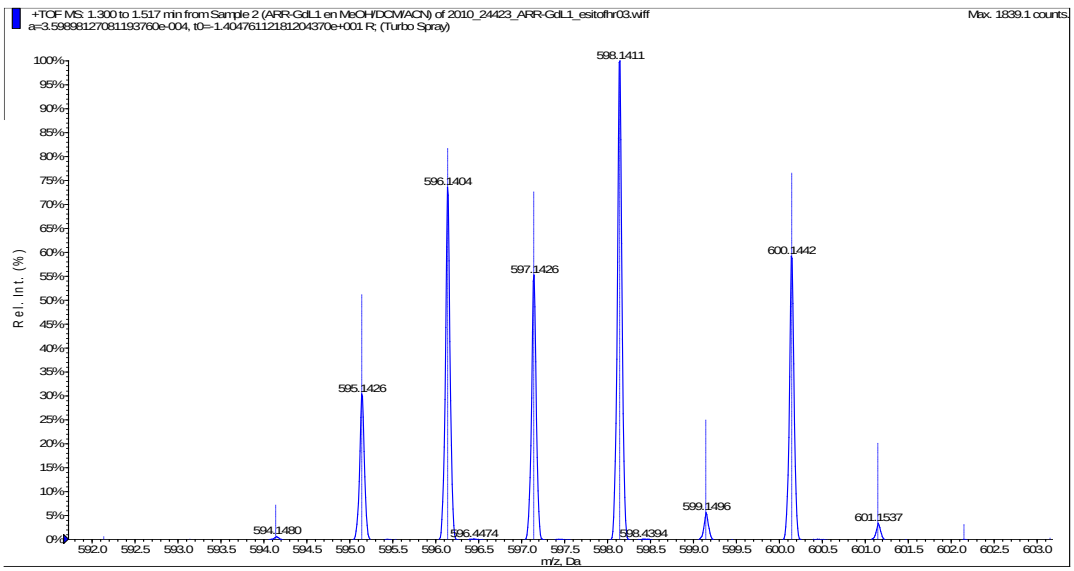


[Eu(Me_2dodpa)]OTf

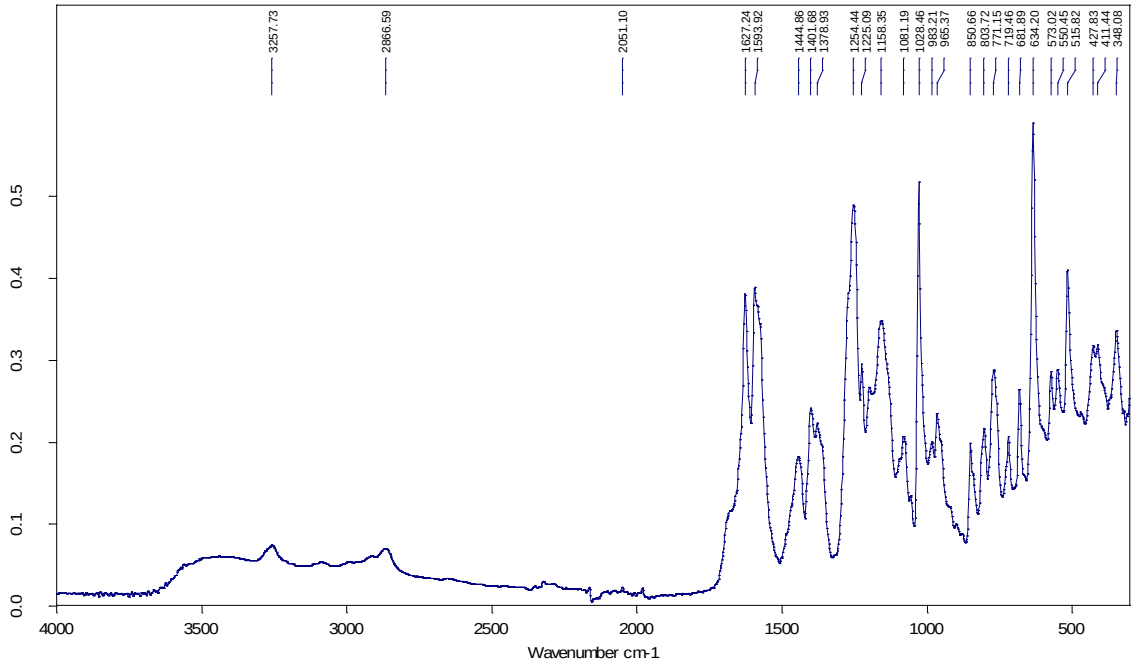
Espectro de masas ESI^+



Espectro ESI^+ HR



Espectro IR


3257.73
2866.59
2051.10
1627.24
1593.92
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1401.68
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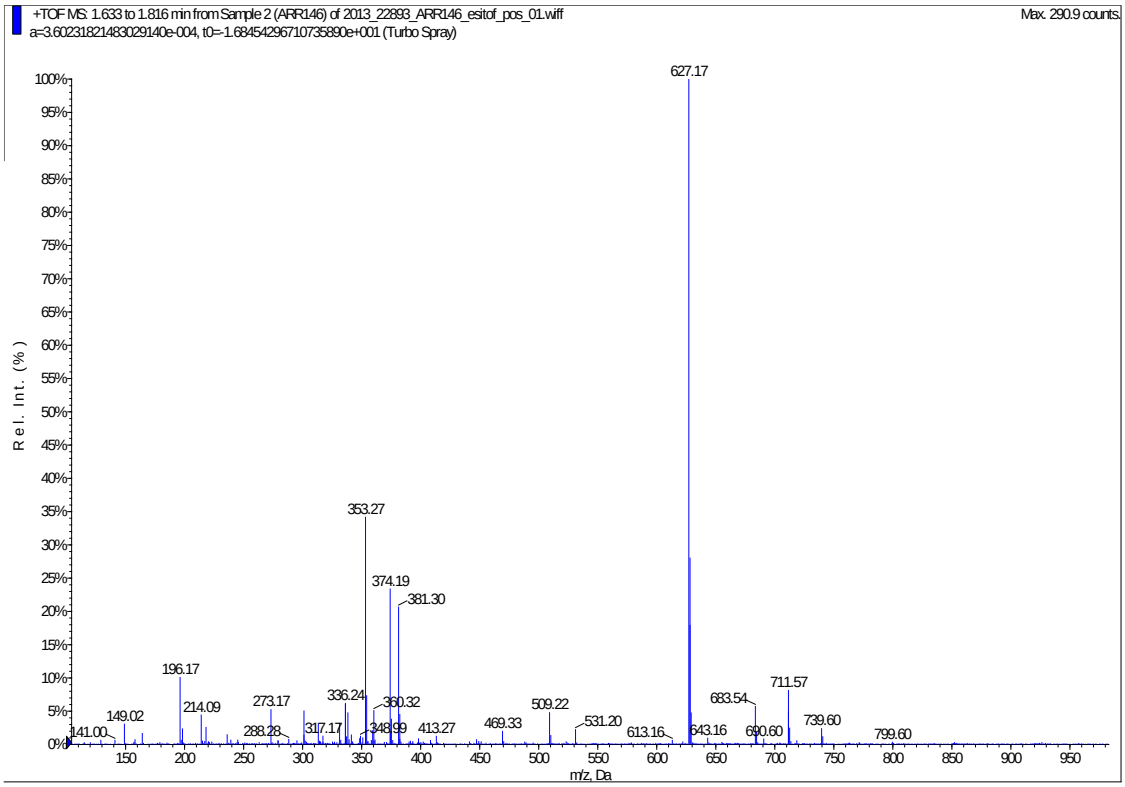
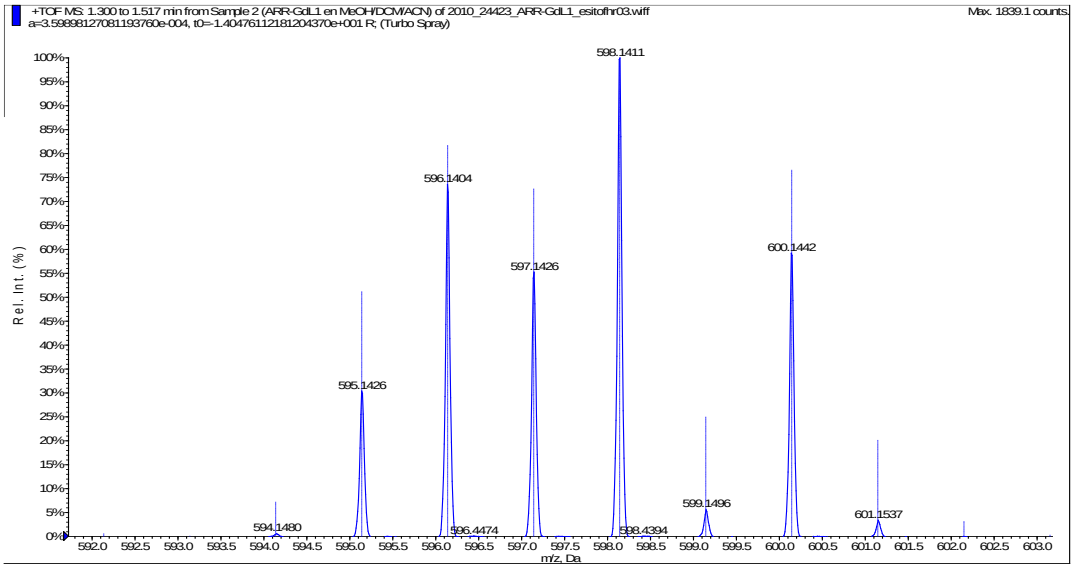
1254.44
1225.09
1158.35
1081.19
1028.46
983.21
965.37
850.66
803.72
771.15
719.46
681.89
634.20
573.02
550.45
515.82
427.83
411.44
348.08
0.0
0.1
0.2
0.3
0.4
0.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(Me$_2$dodpa)]OTf

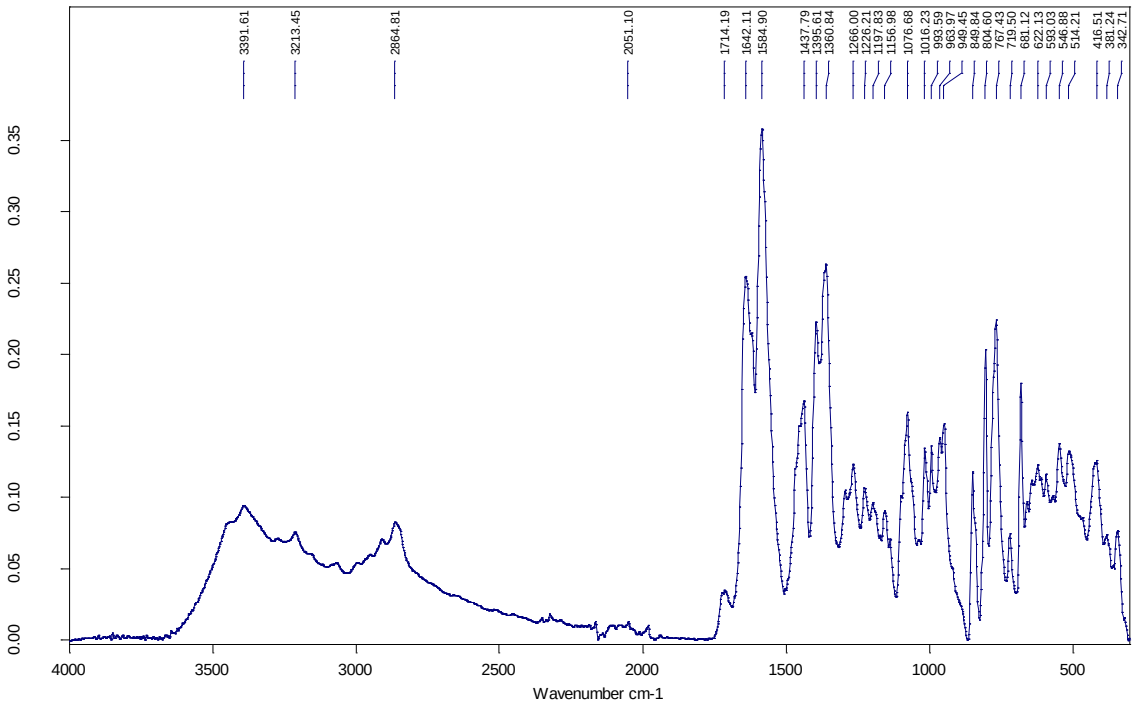
Espectro de masas ESI$^+$



Espectro ESI$^+$ HR



Espectro IR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967.07
949.45
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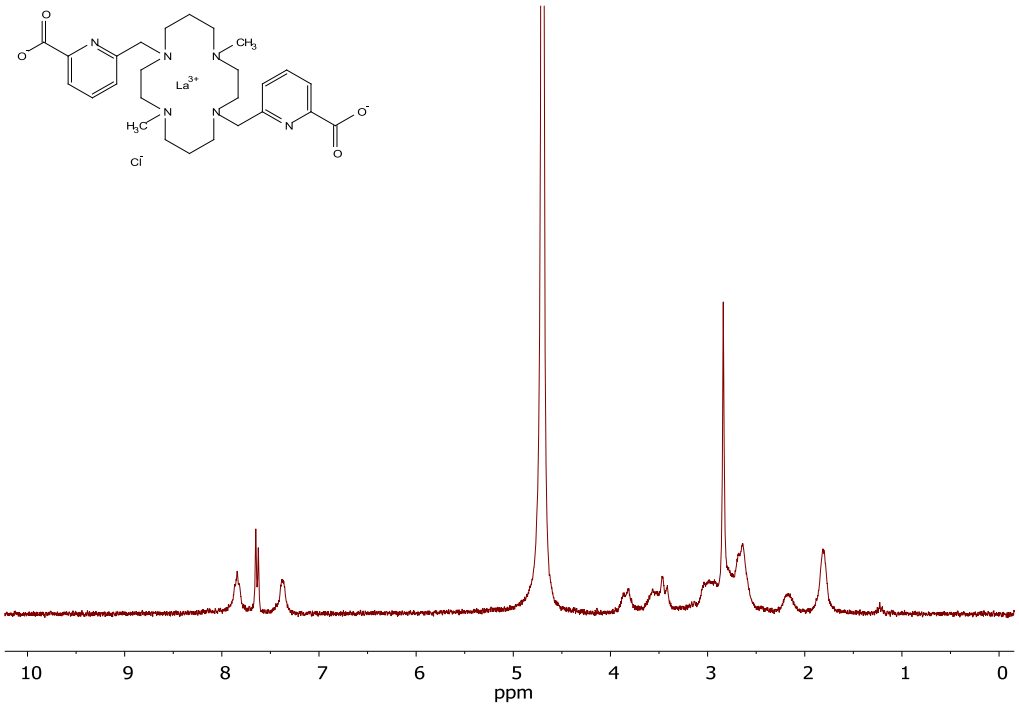
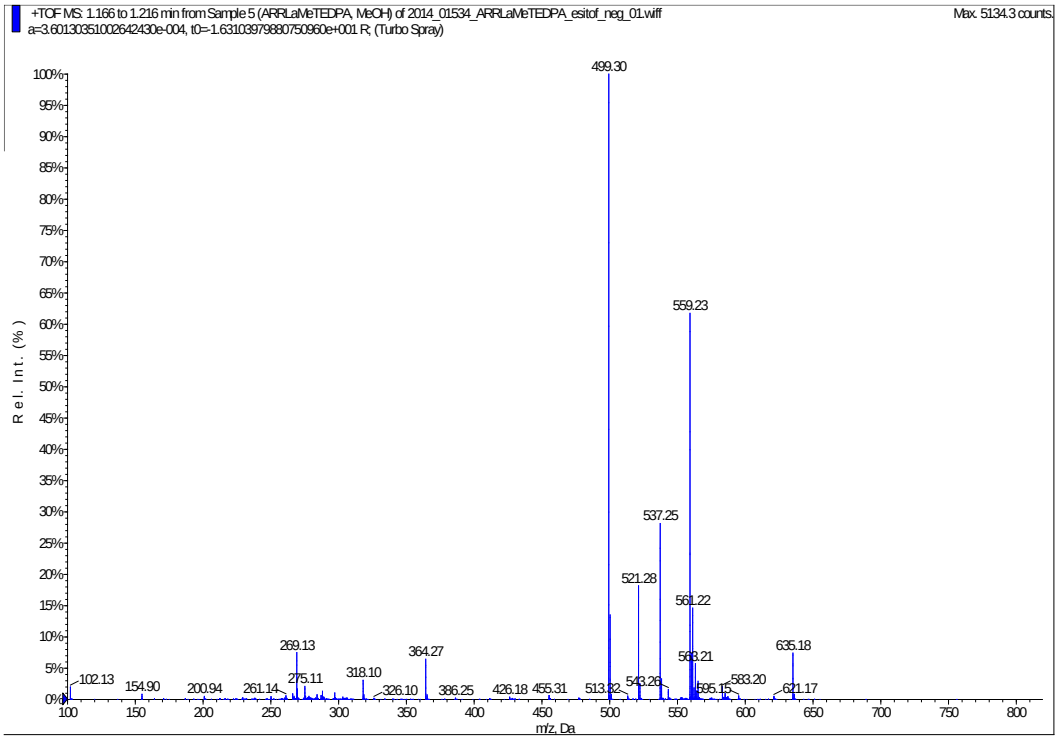
804.60
767.43
719.50
681.12
622.13
593.03
546.88
514.21
416.51
381.24
342.71
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[La(Me$_2$tedpa)]Cl

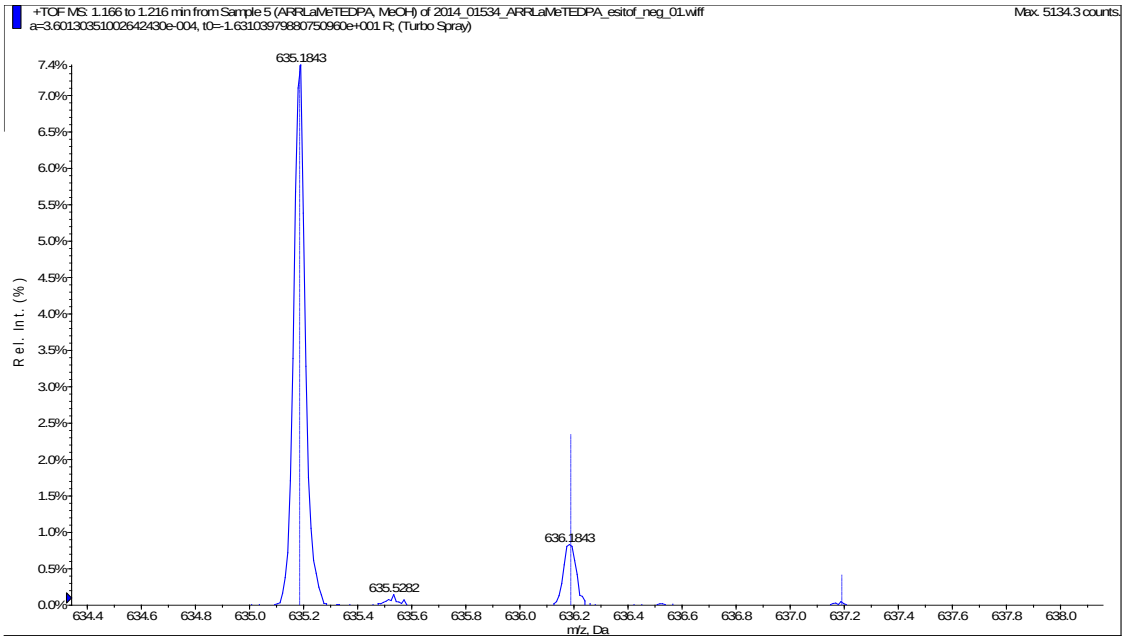
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



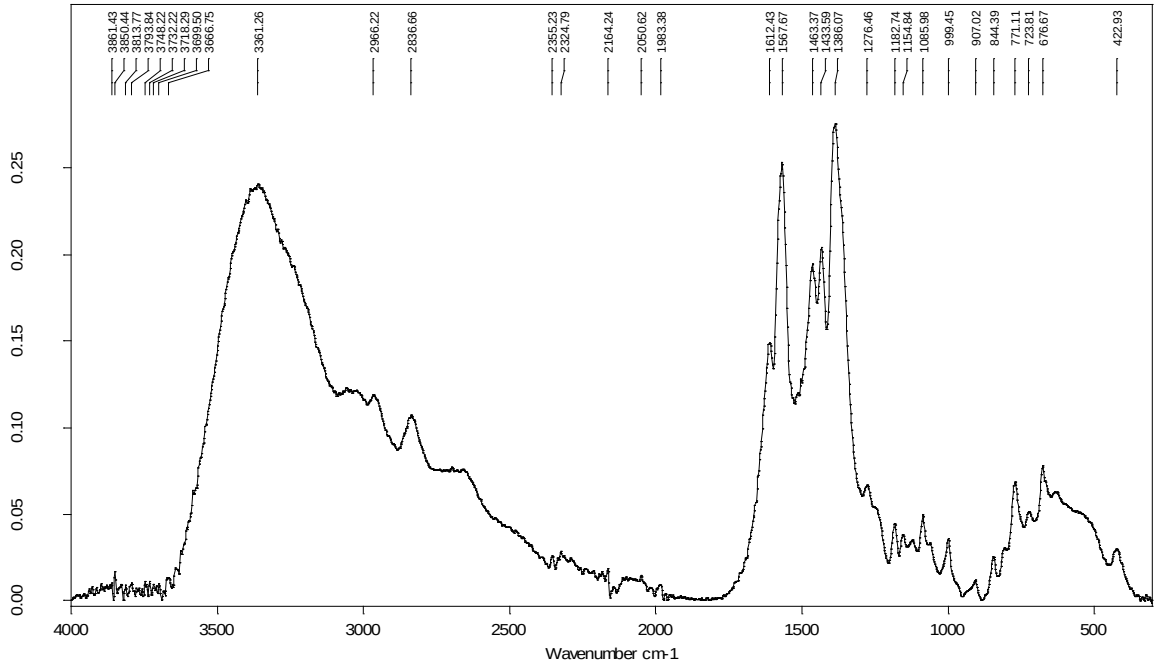
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

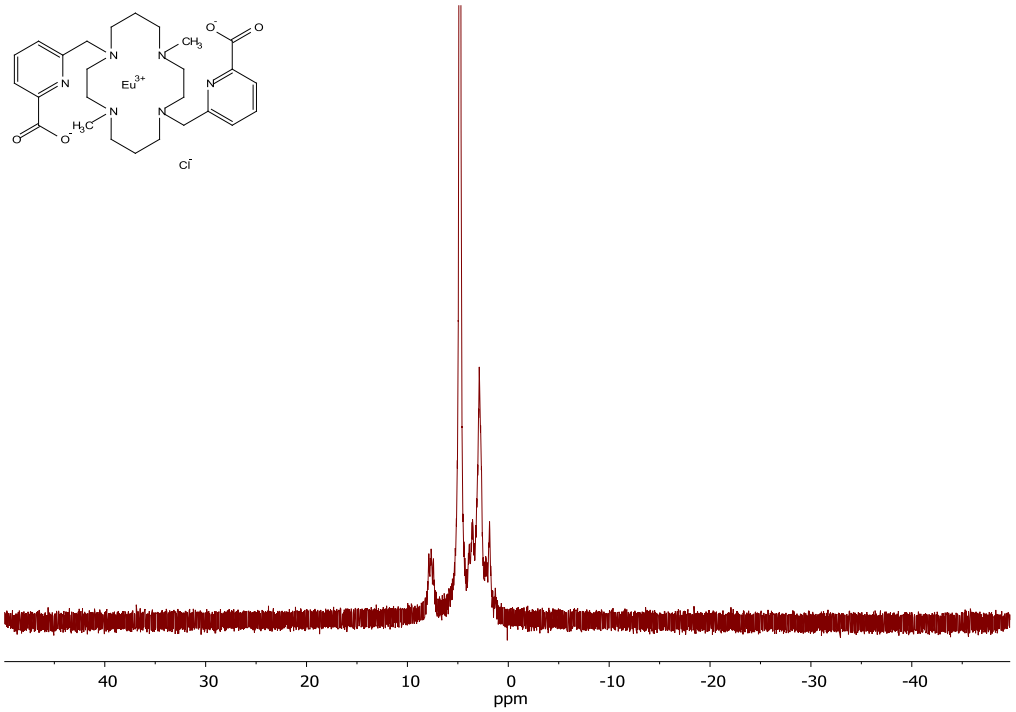


Espectro IR

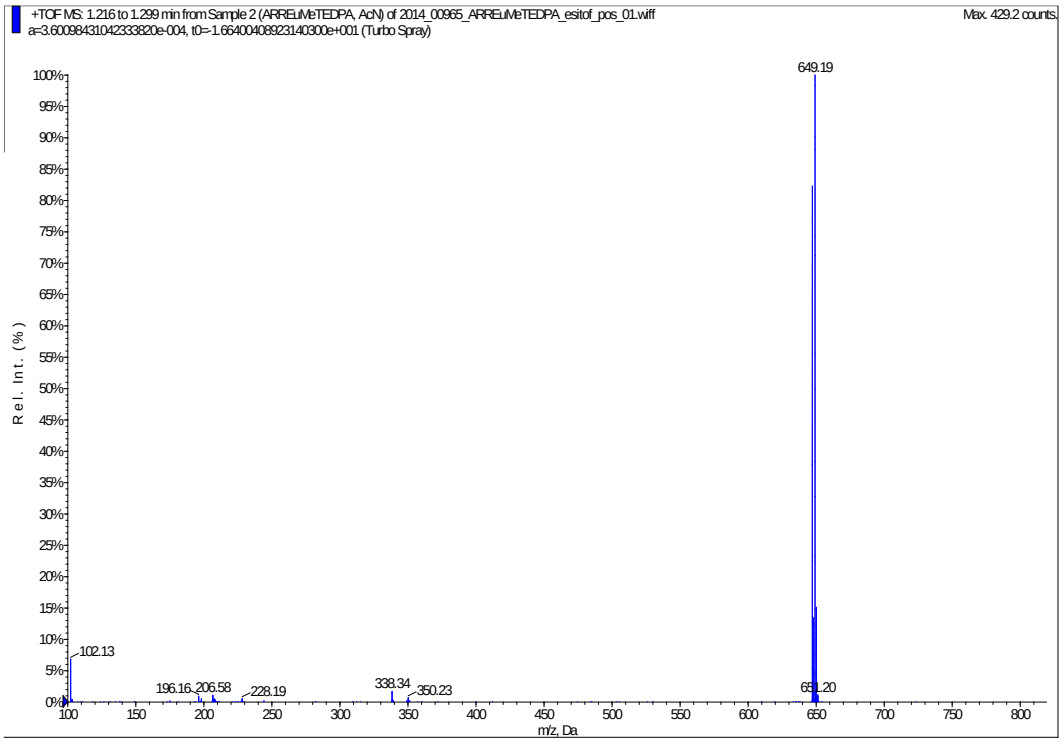


[Eu(Me$_2$tedpa)]Cl

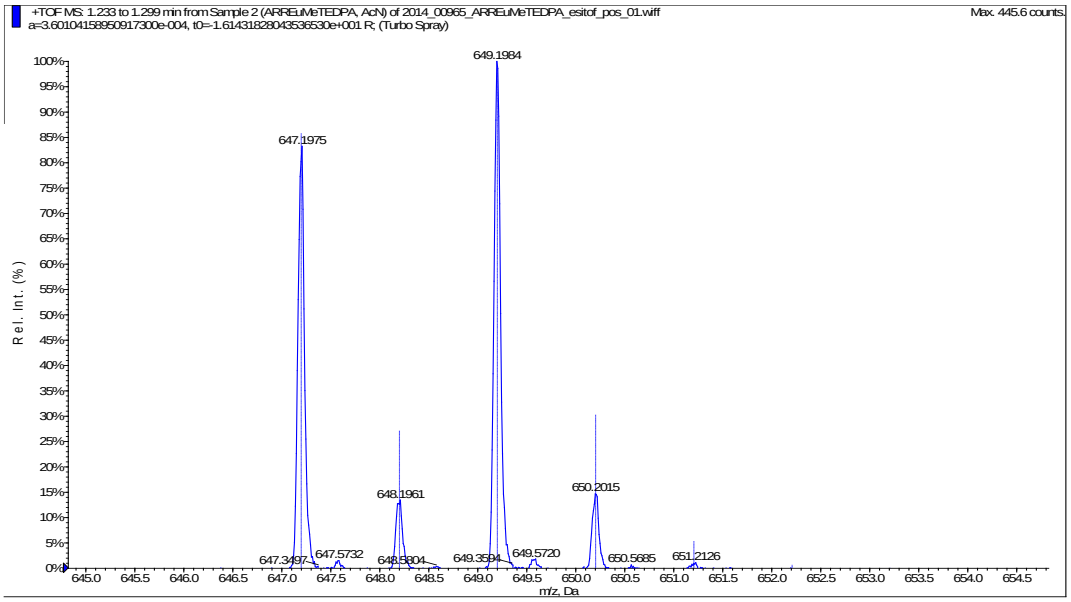
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



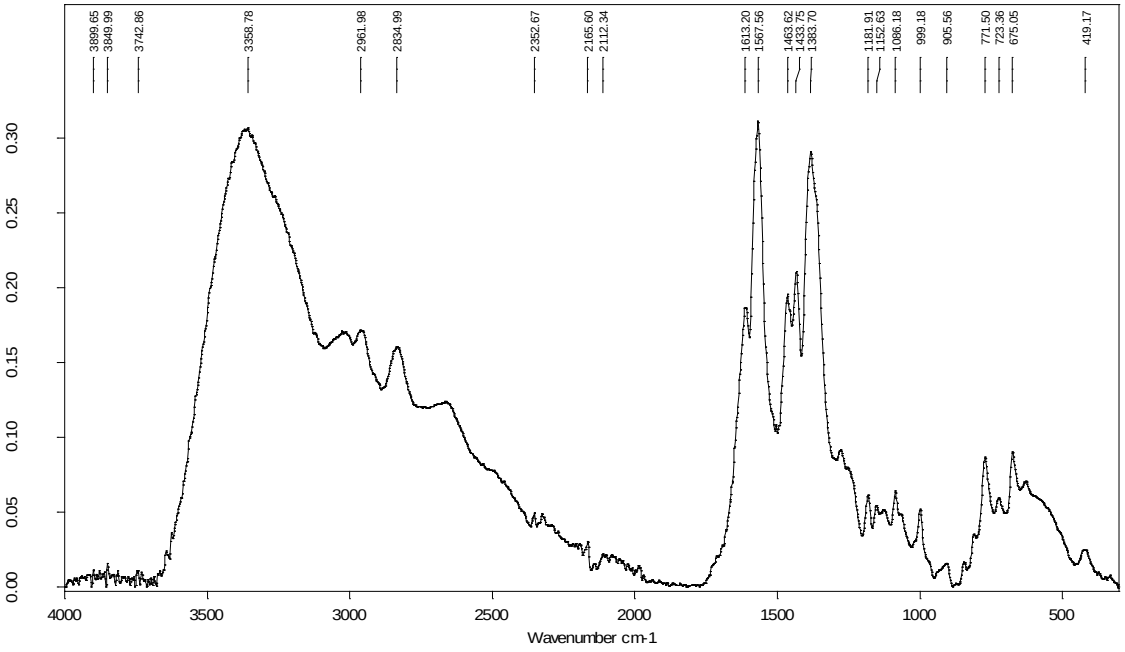
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

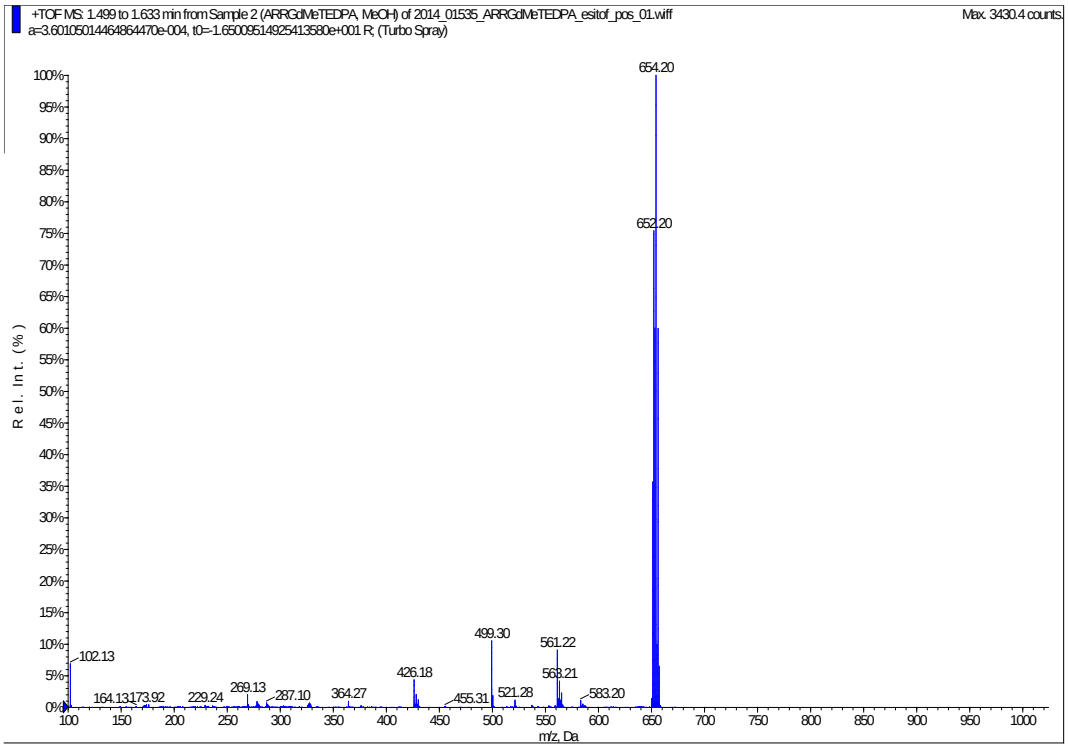


Espectro IR

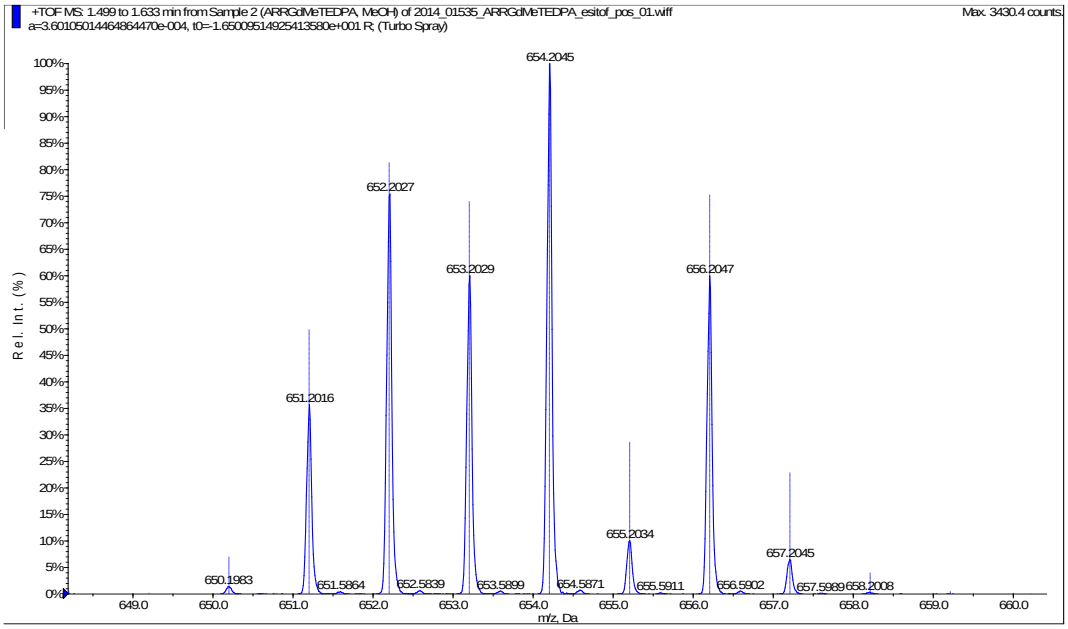


[Gd(Me$_2$tedpa)]Cl

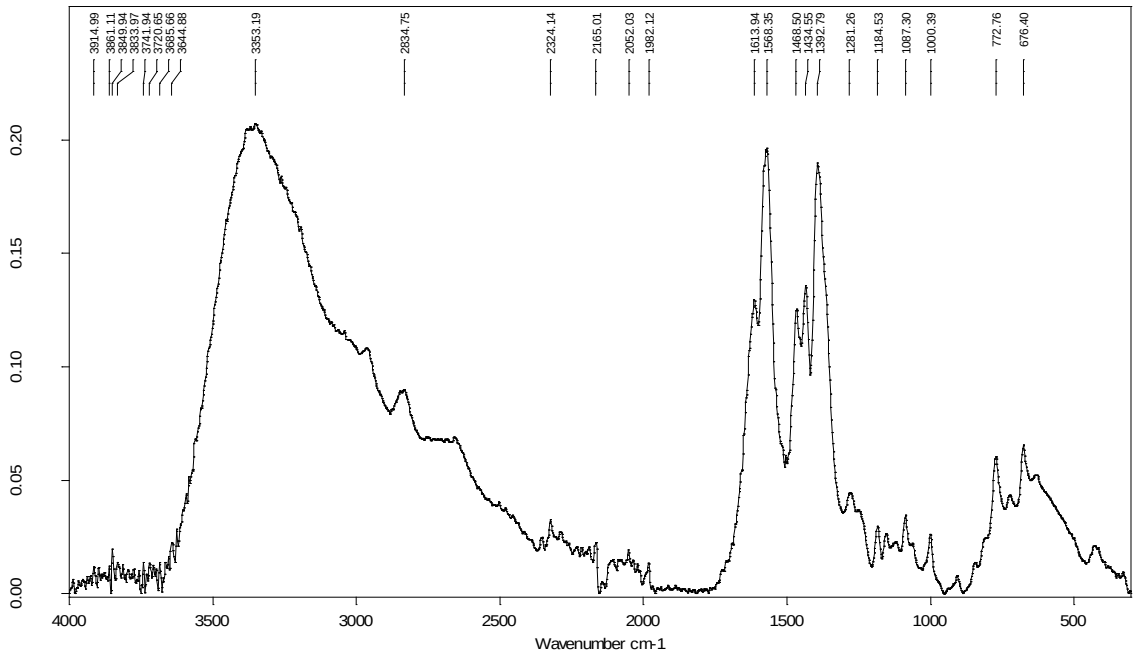
Espectro de masas ESI$^+$



Espectro ESI$^+$ HR



Espectro IR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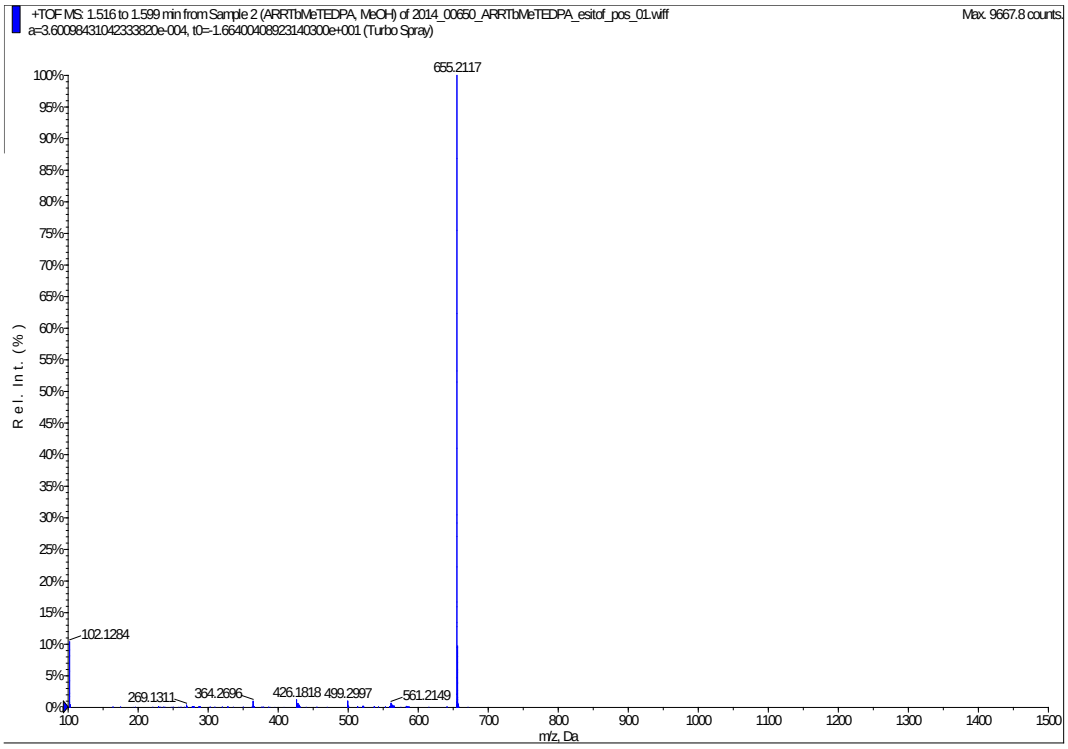
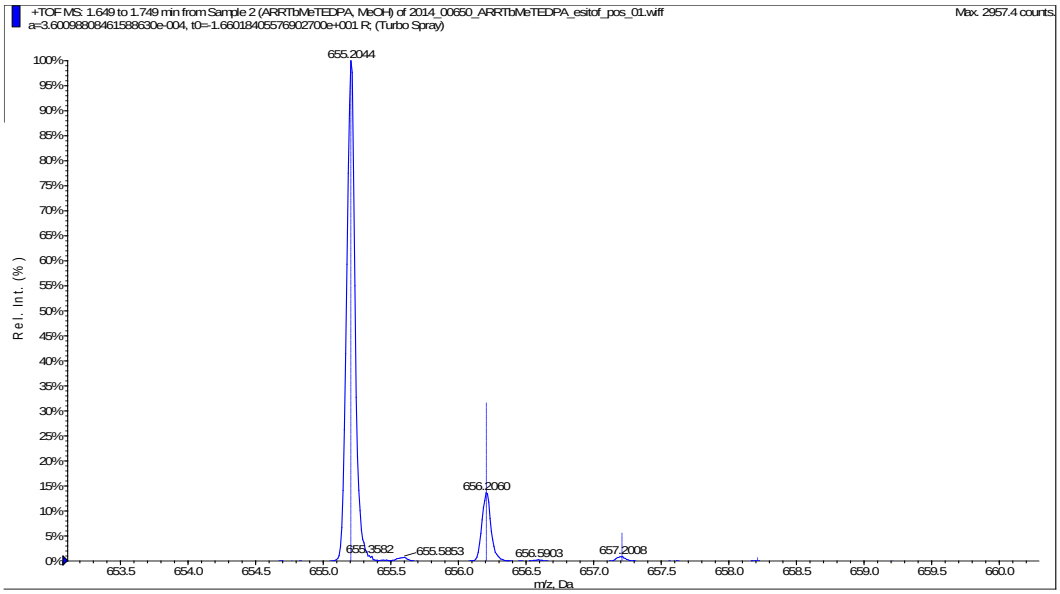
2324.14
2165.01
2052.03
1982.12
1613.94
1568.35
1468.50
1434.55
1392.79
1281.26
1184.53
1087.30
1000.39
772.76
676.40
0.00
0.05
0.10
0.15
0.20
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(Me$_2$tedpa)]Cl

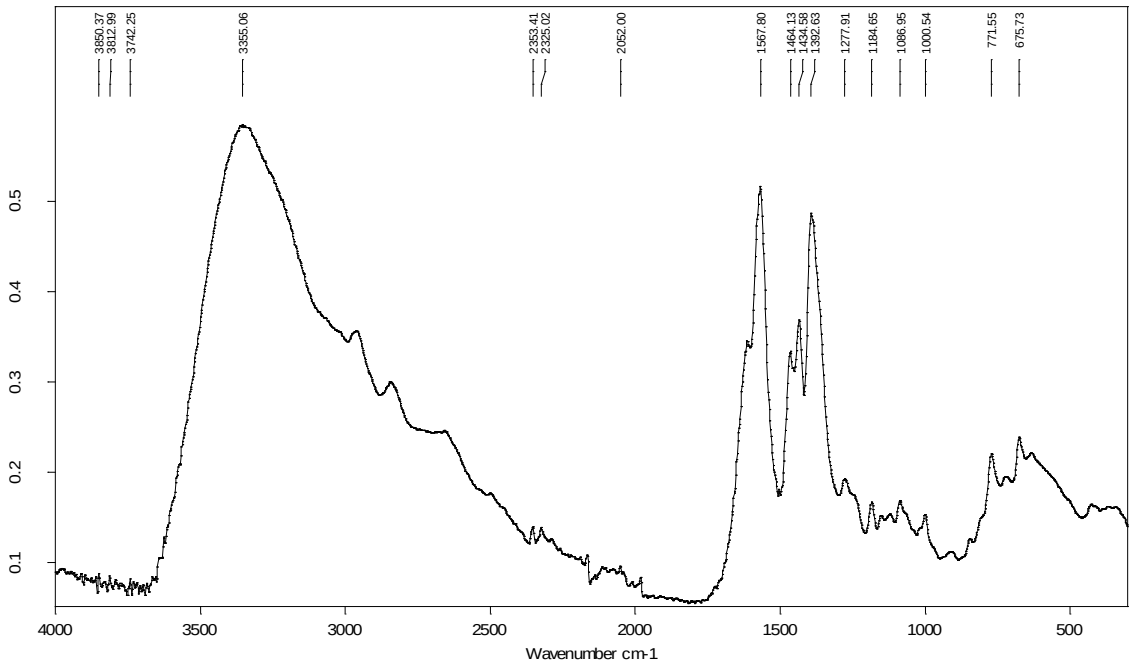
Espectro de masas ESI$^+$



Espectro ESI$^+$ HR



Espectro IR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2052.00
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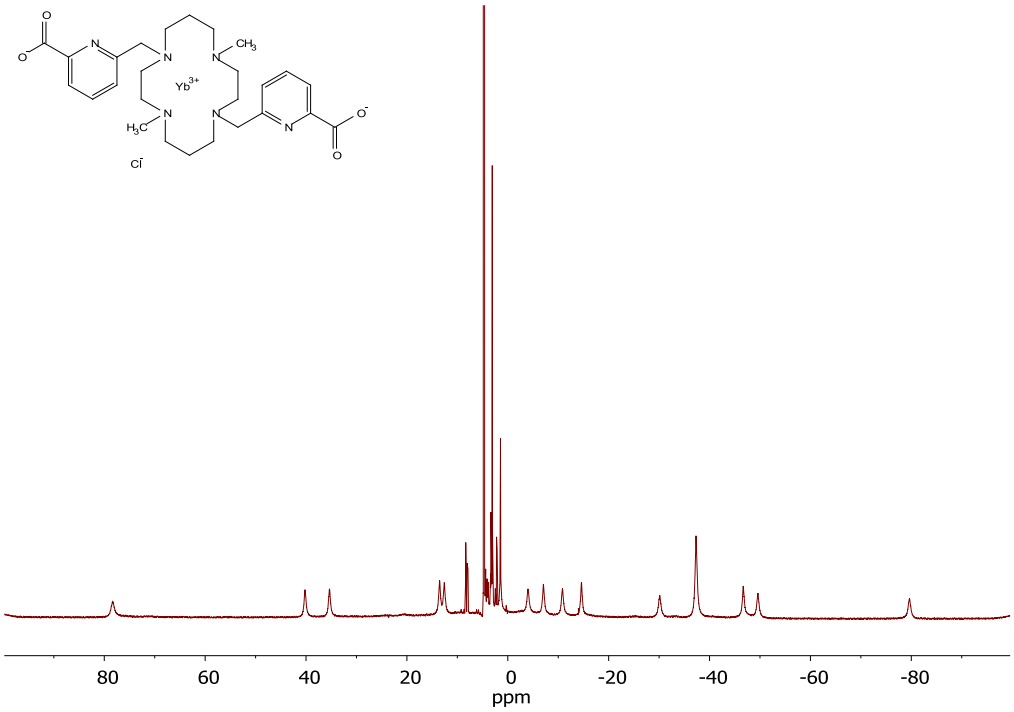
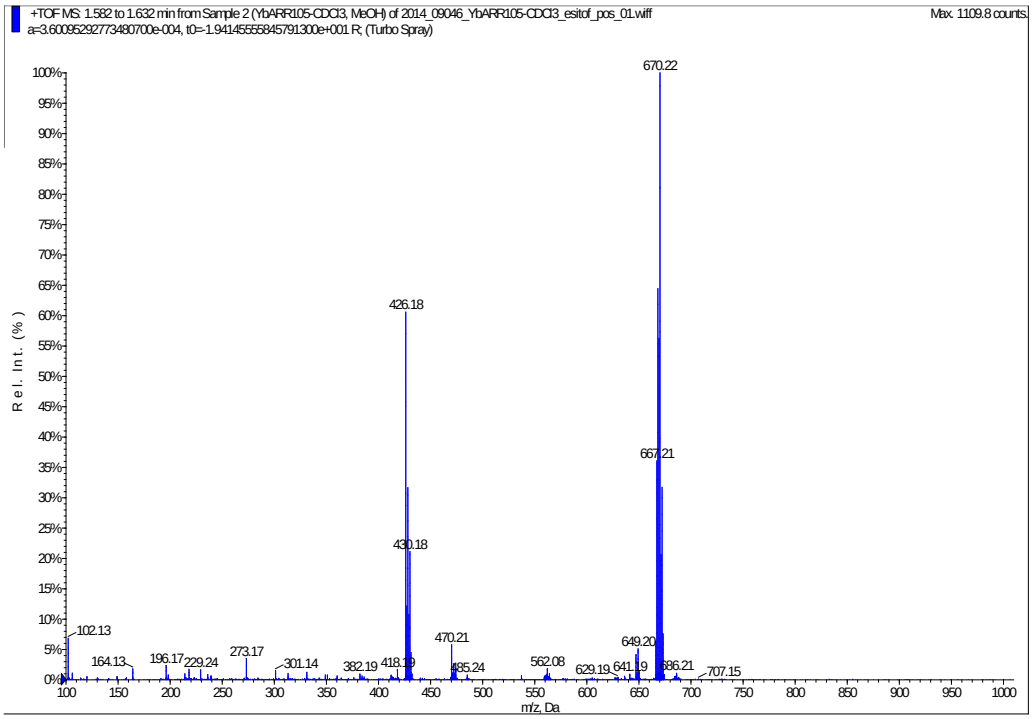
1392.63
1277.91
1184.65
1086.95
1000.54
771.55
675.73
0.1
0.2
0.3
0.4
0.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Yb(Me$_2$tedpa)]Cl

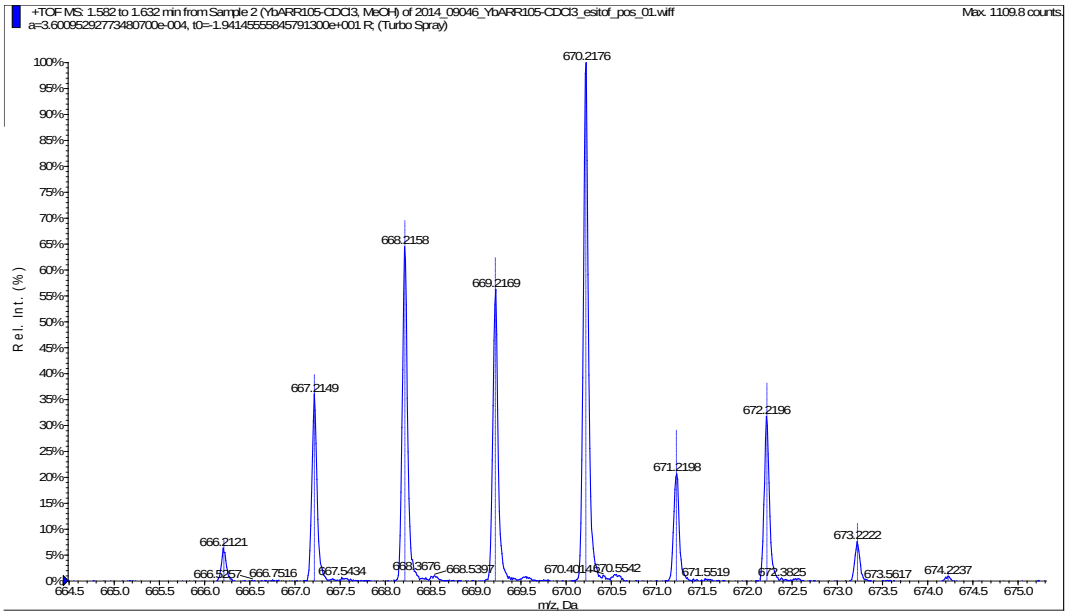
^{1}H-RMN (D_2O, 278K, 300 MHz) (δ/ppm)



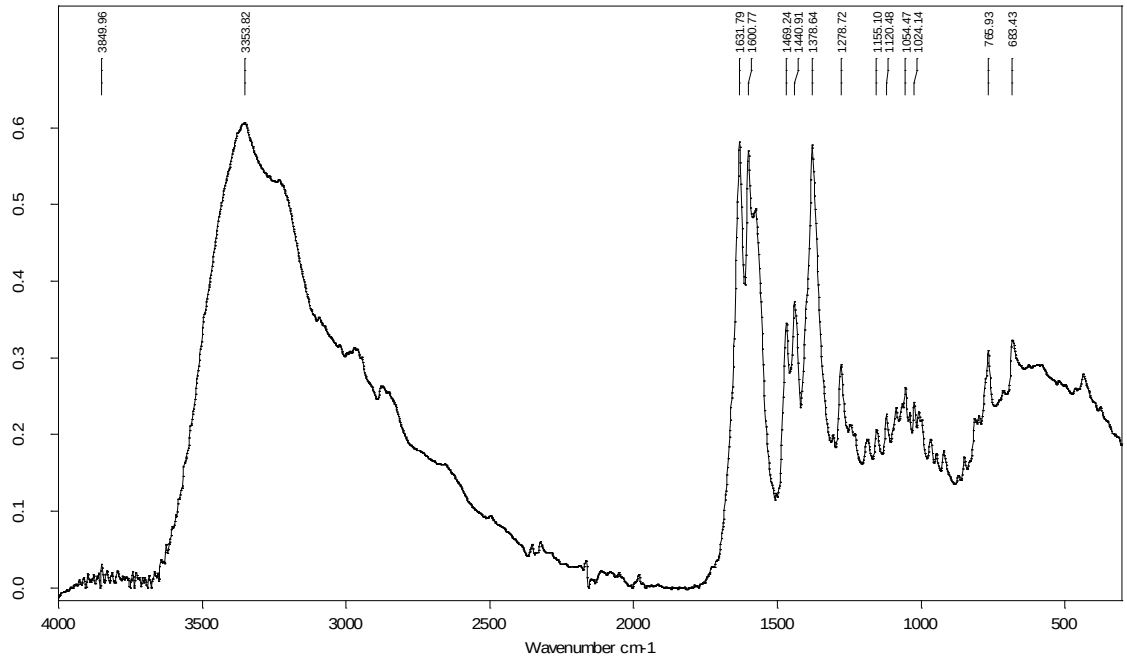
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

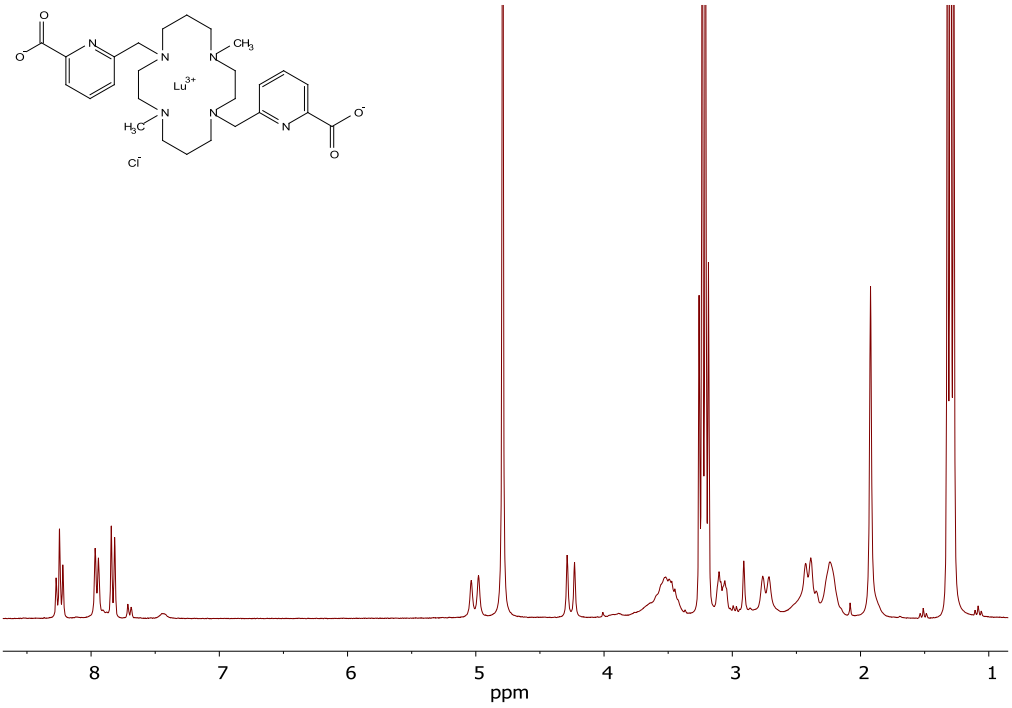


Espectro IR

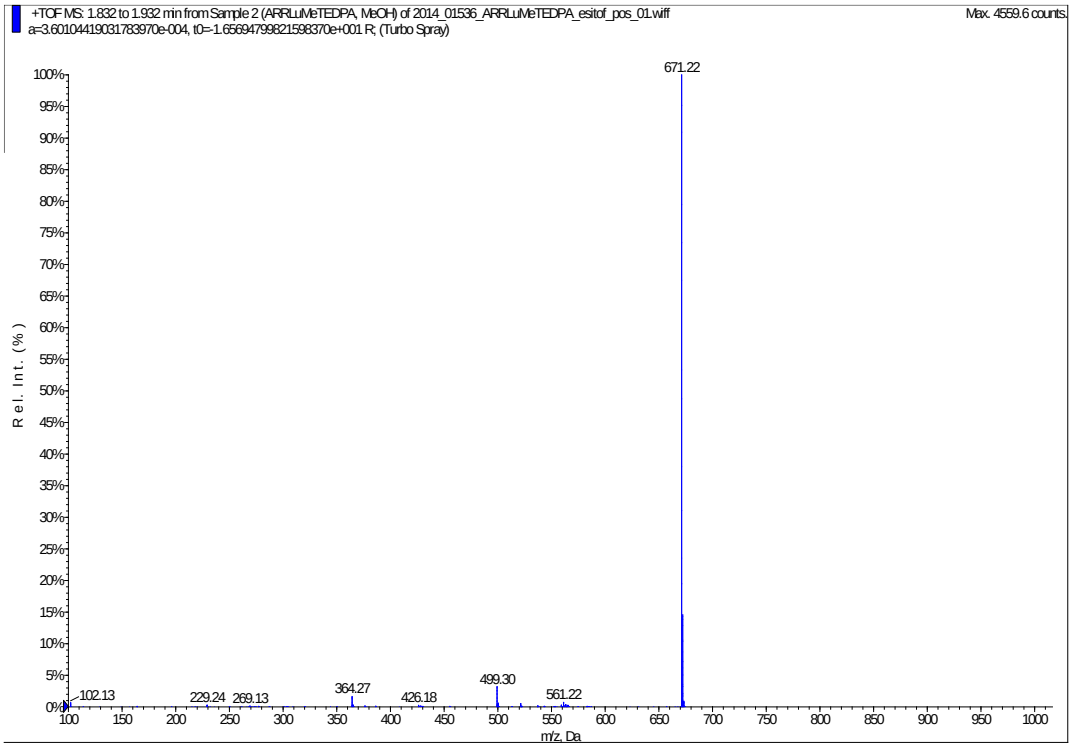


[Lu(Me$_2$tedpa)]Cl

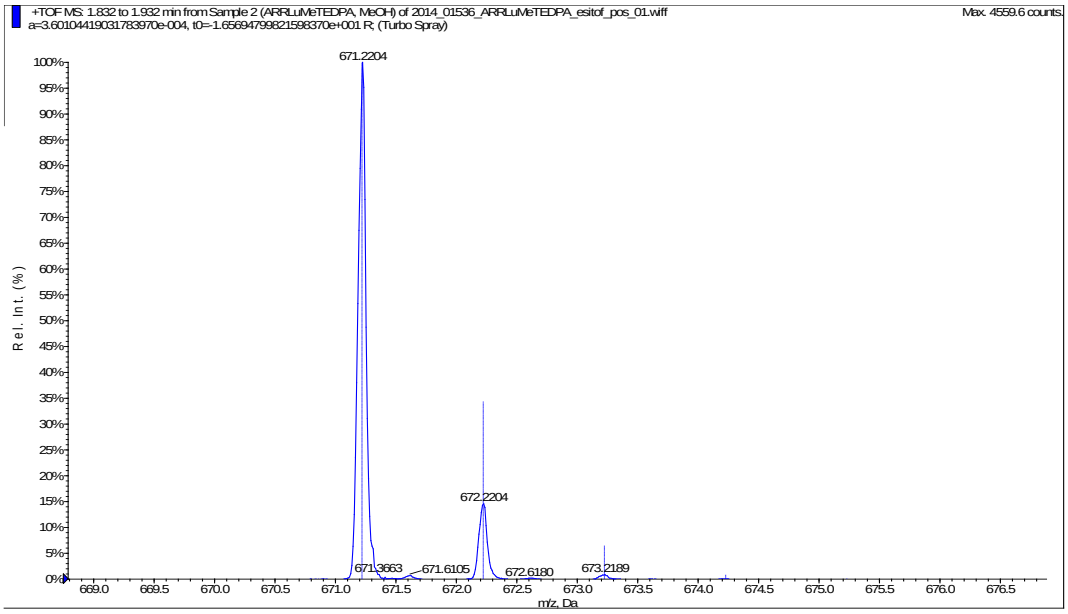
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



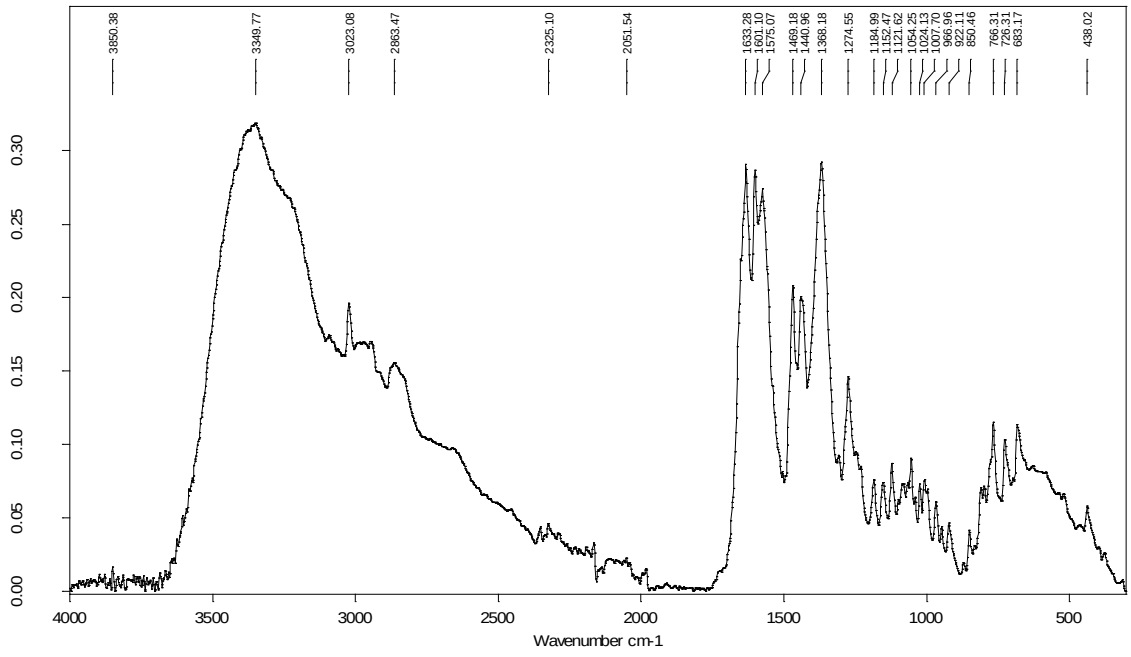
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

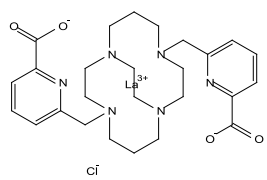


Espectro IR

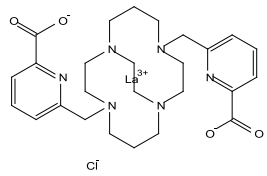


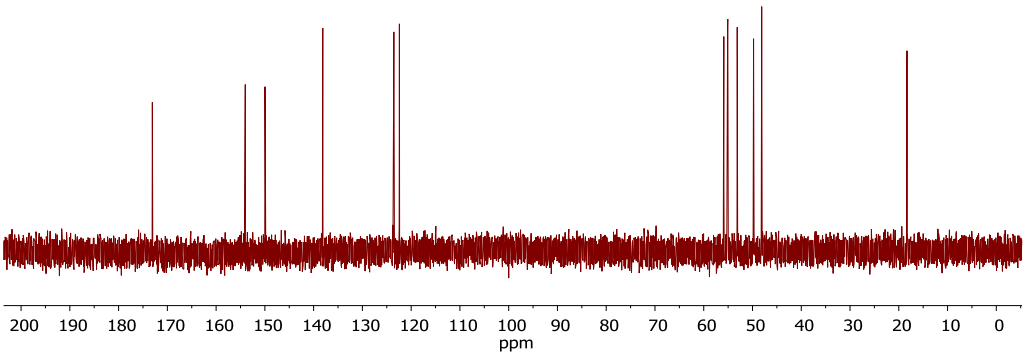
[La(cb-tedpa)]Cl

^{1}H-RMN (D_2O, 500 MHz) (δ/ppm)

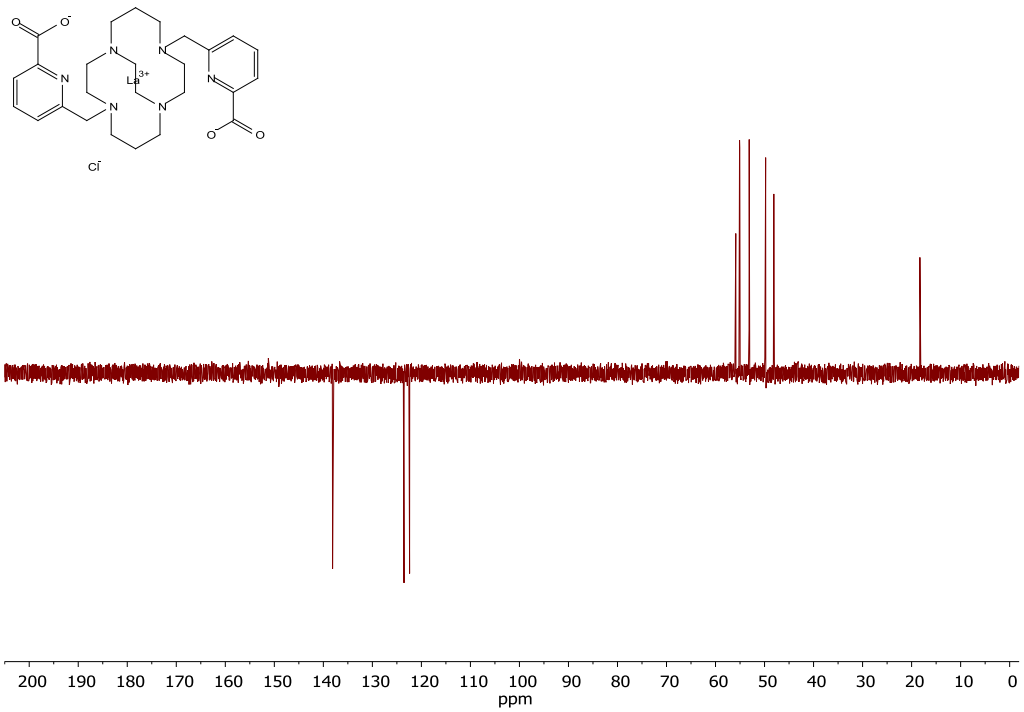


^{13}C-RMN (D_2O, 125,8 MHz) (δ/ppm)

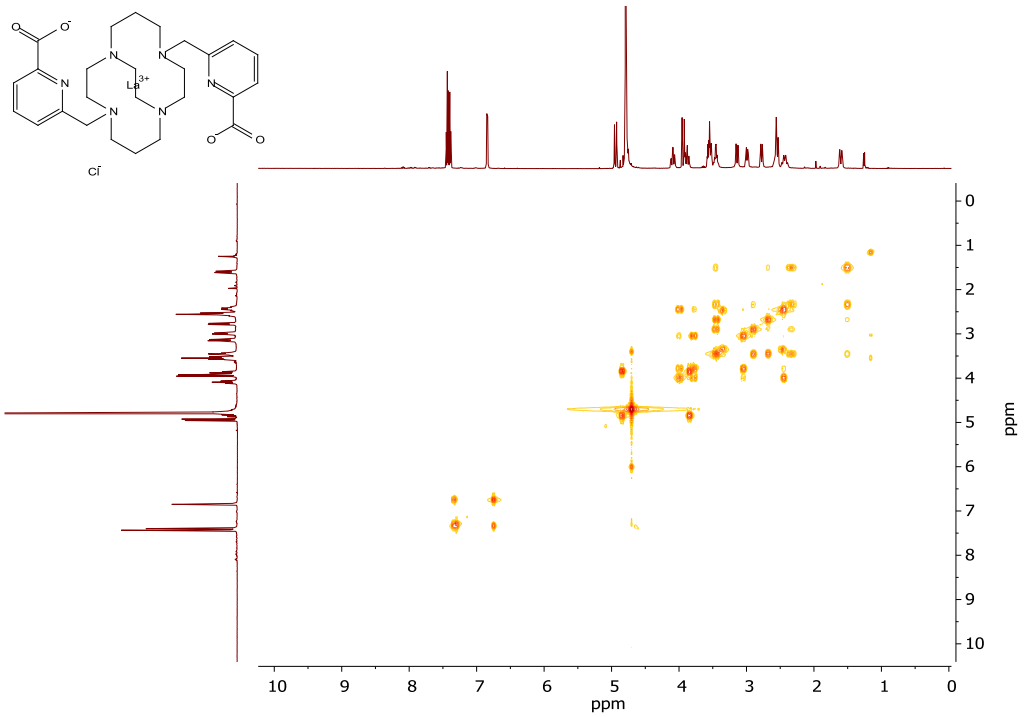




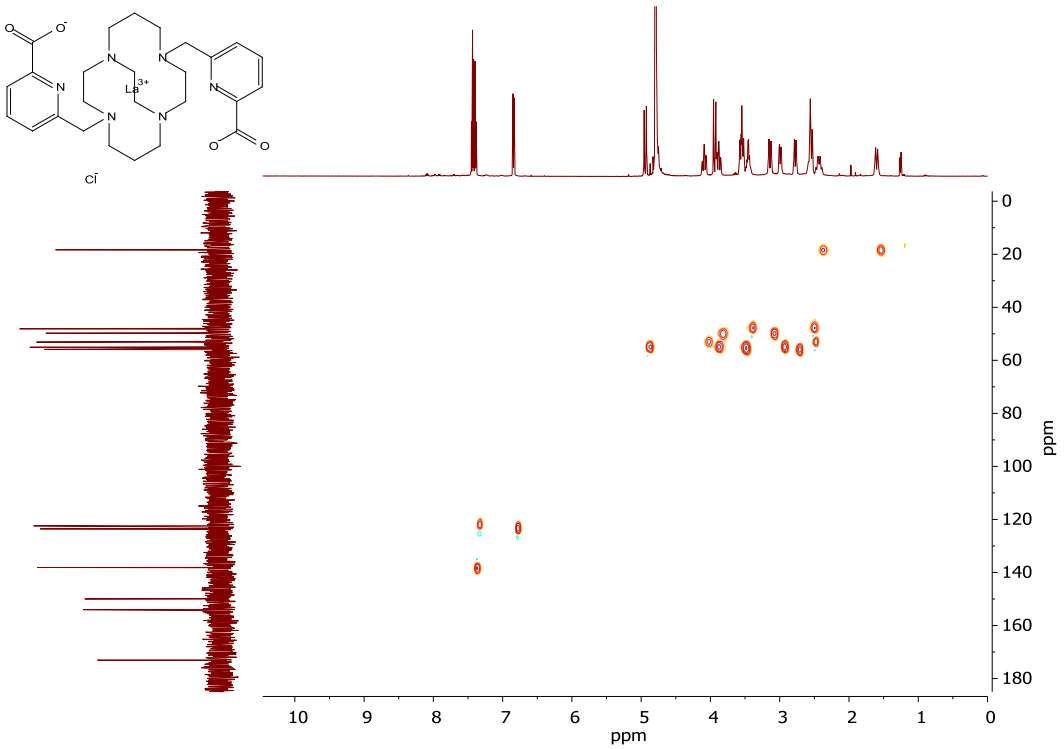
DEPT-RMN (D_2O) (δ/ppm)



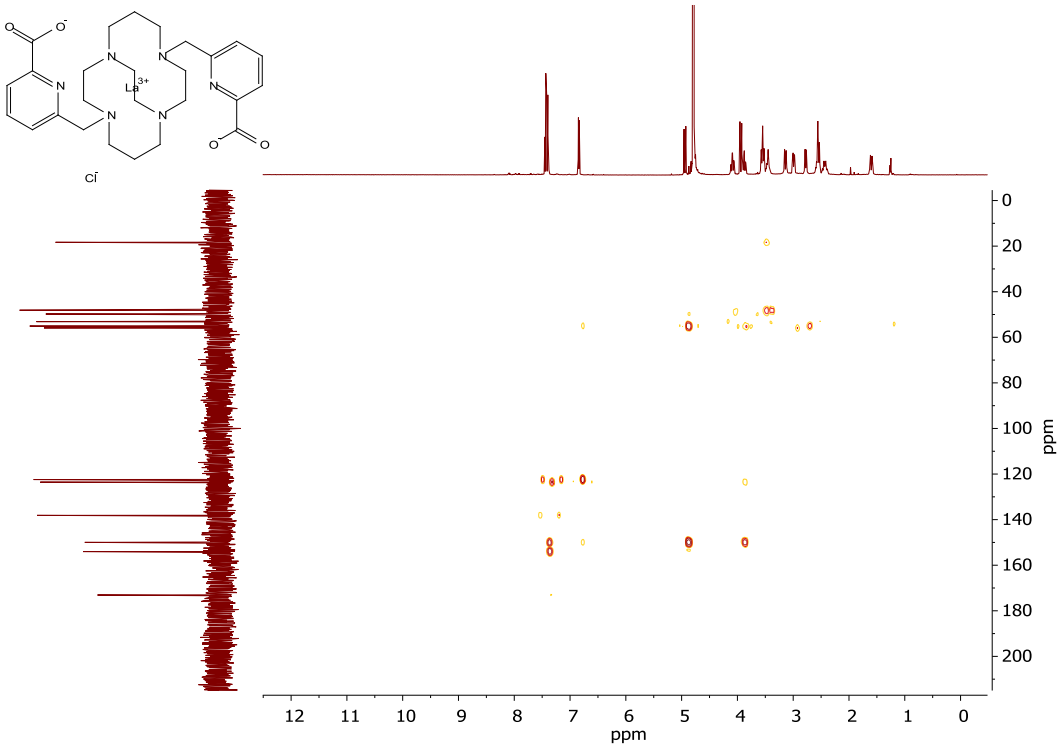
COSY-RMN (D_2O) (δ/ppm)



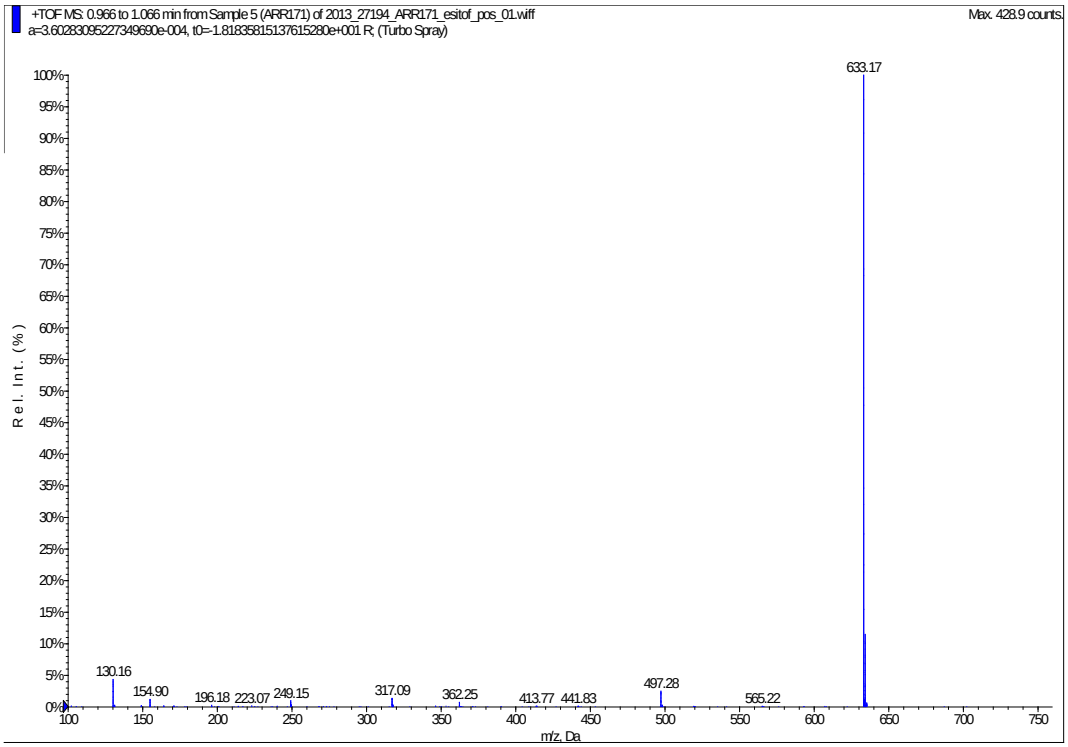
HSQC-RMN (D_2O) (δ/ppm)



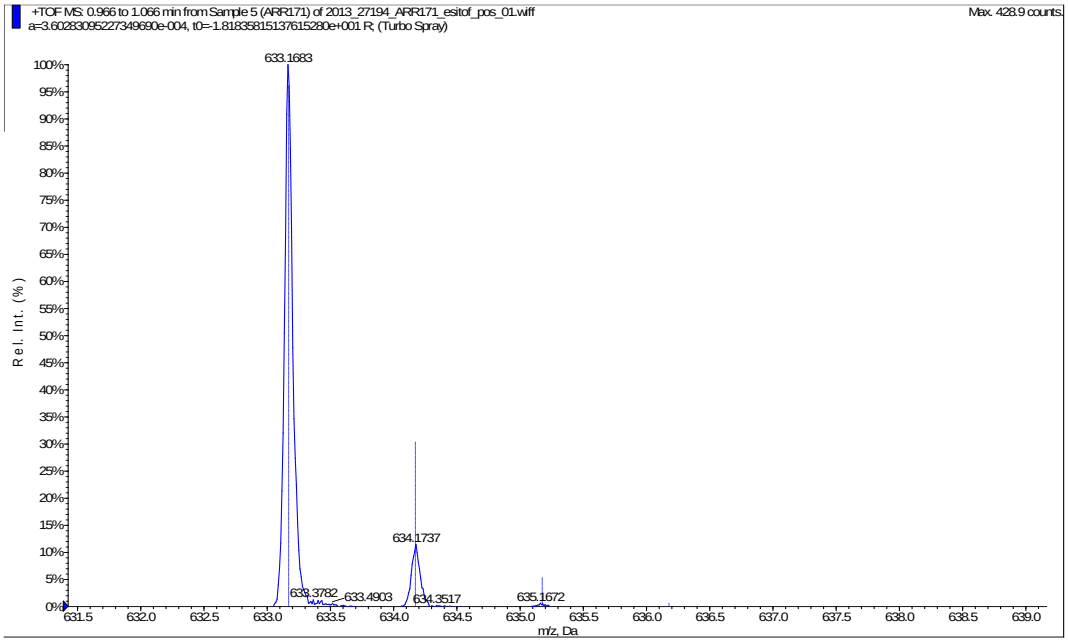
HMBC-RMN (D_2O) (δ/ppm)



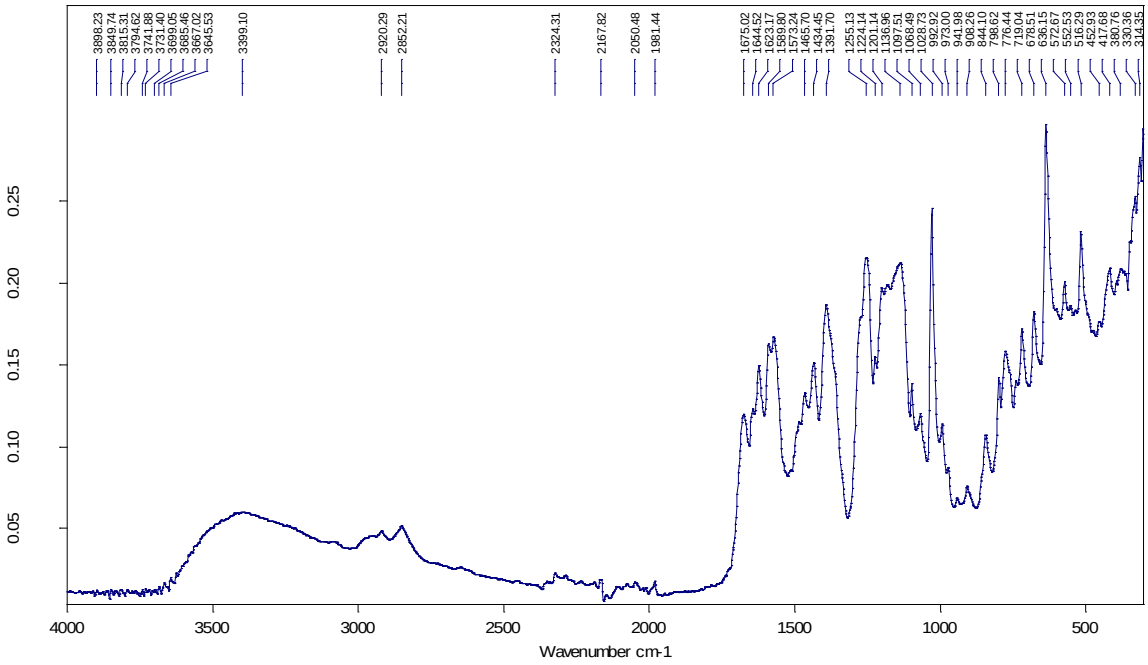
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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798.62
776.44
718.04
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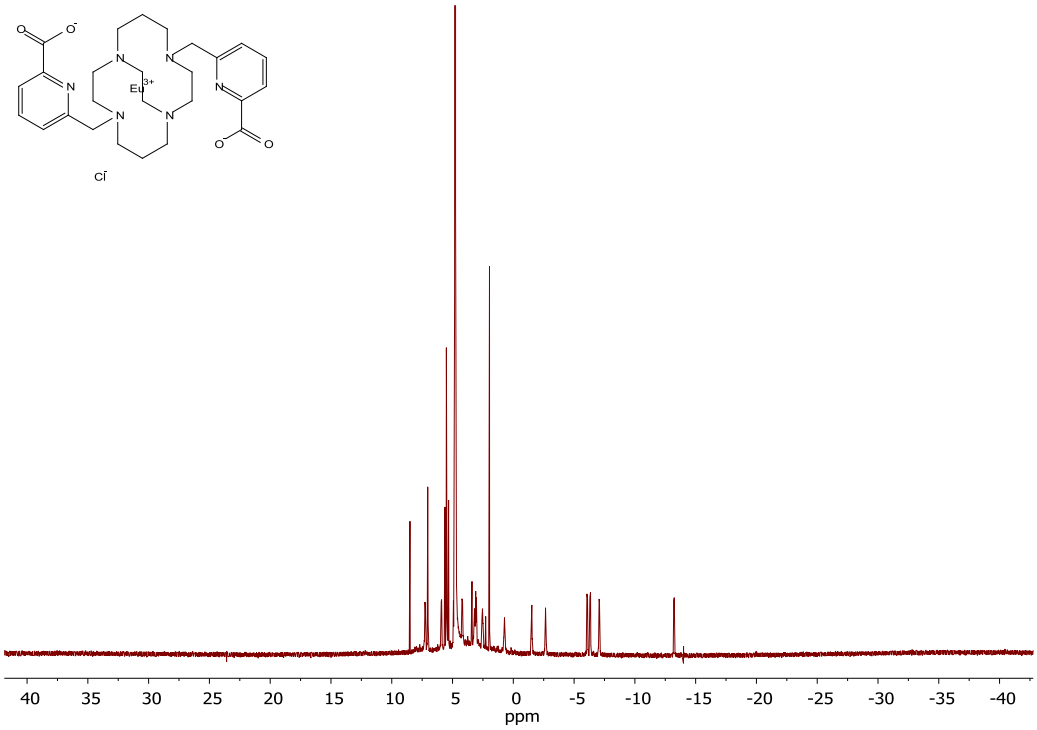
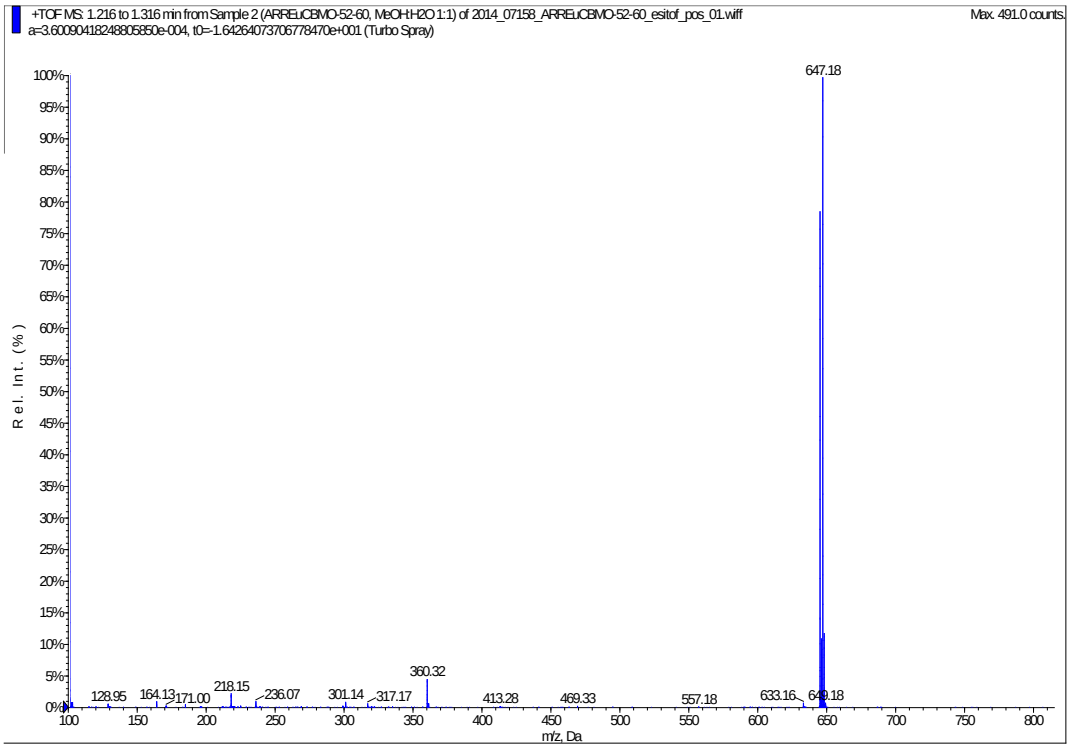
636.15
572.67
552.53
516.29
452.93
437.68
389.76
330.36
314.35
0.25
0.20
0.15
0.10
0.05
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Eu(cb-tedpa)]Cl

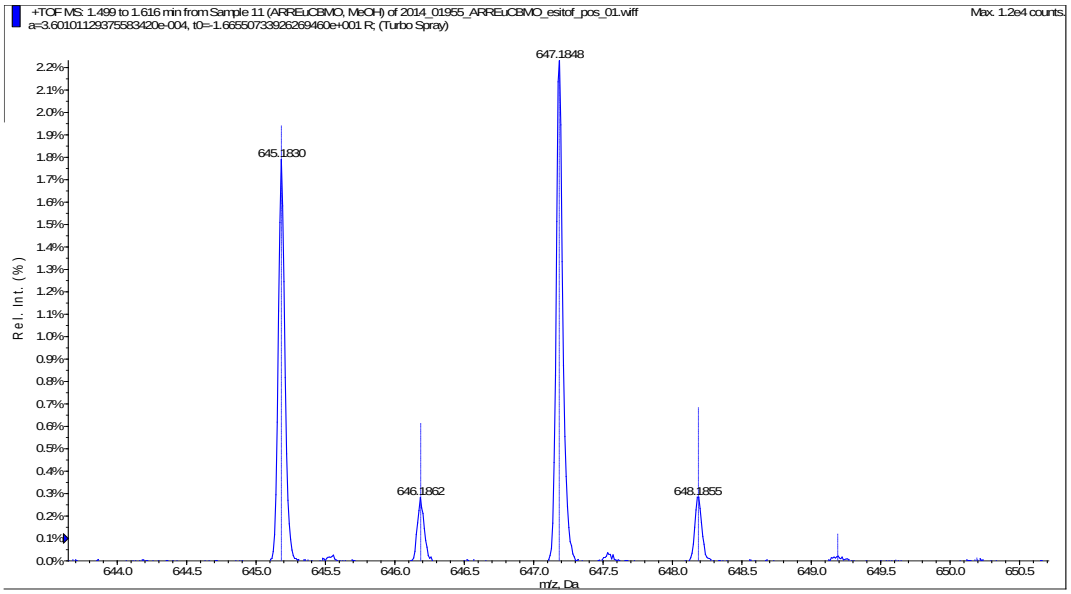
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



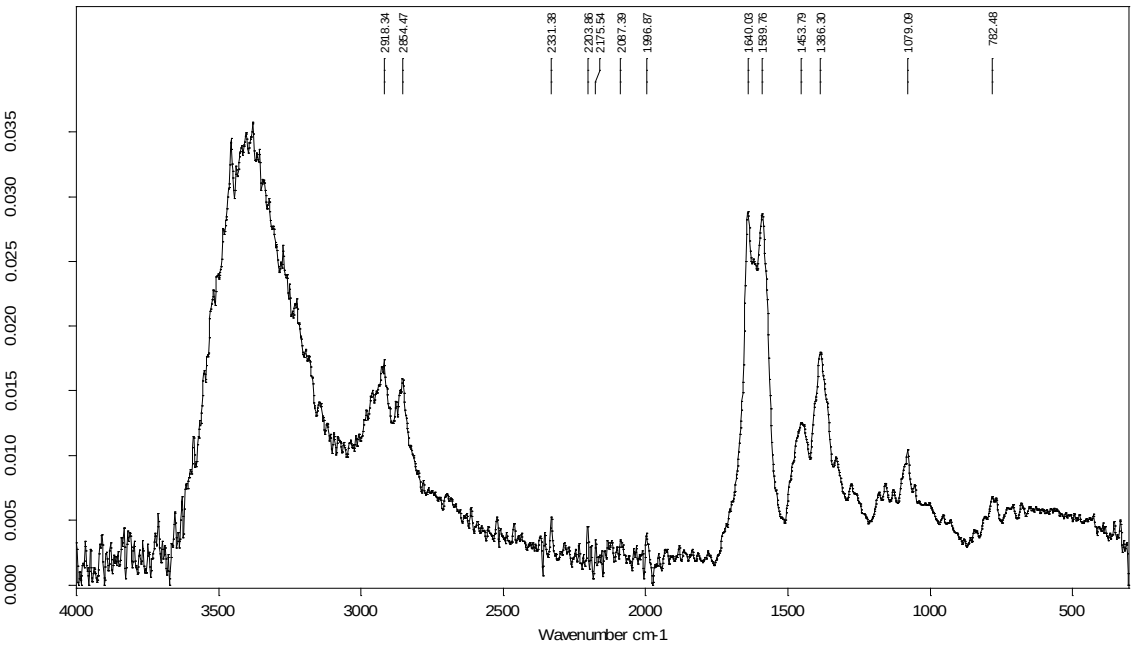
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

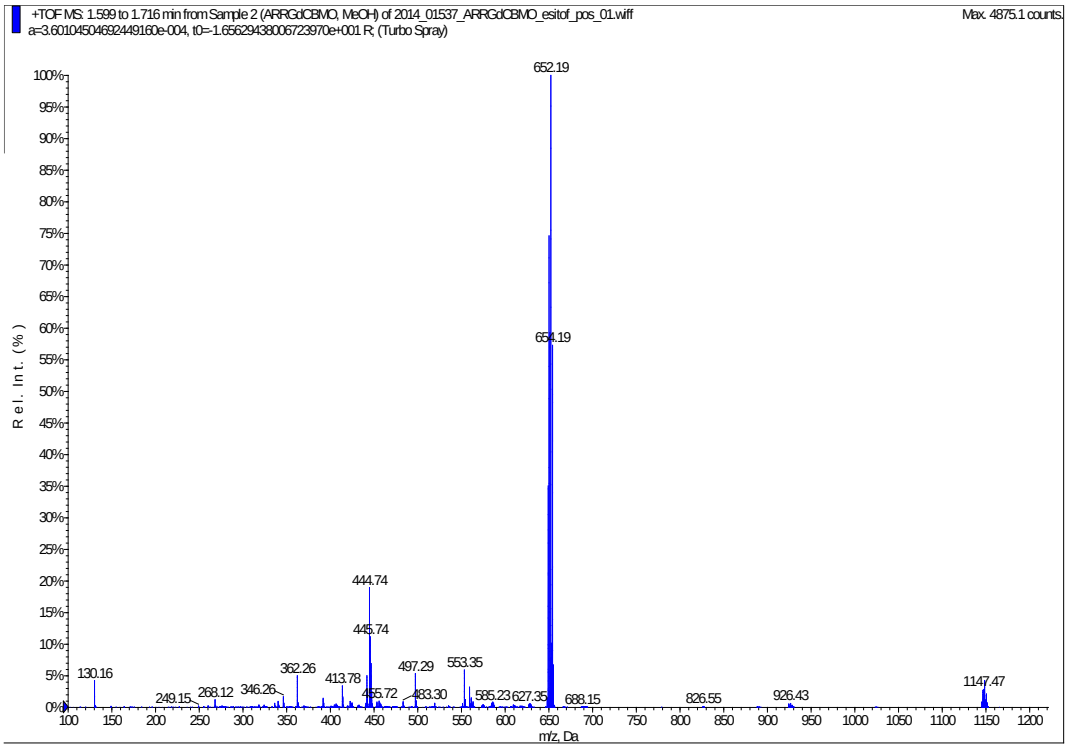


Espectro IR

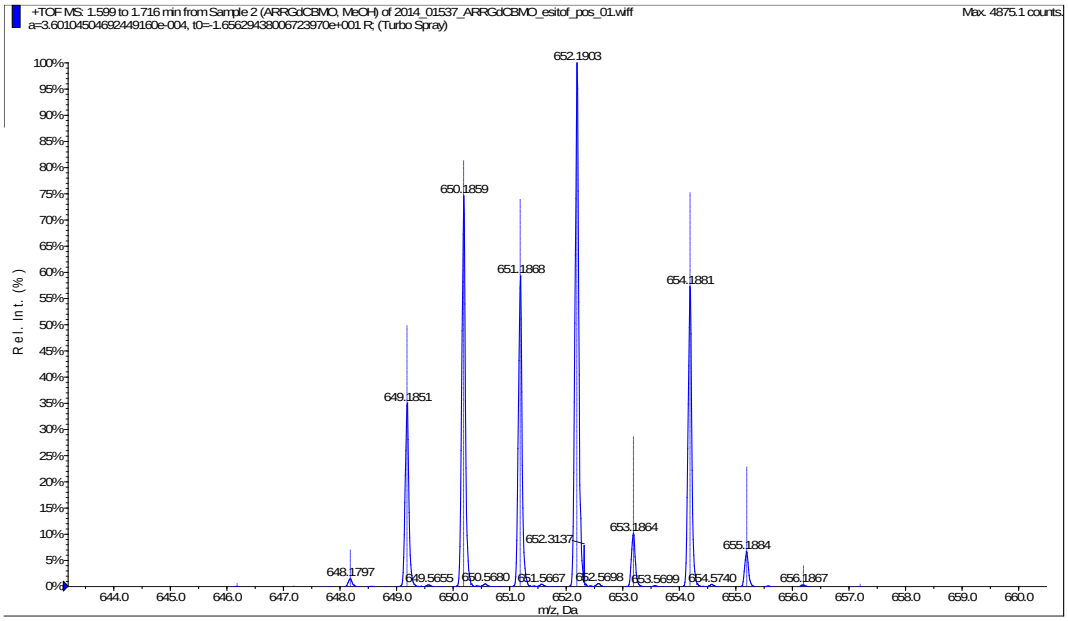


[Gd(cb-tedpa)]Cl

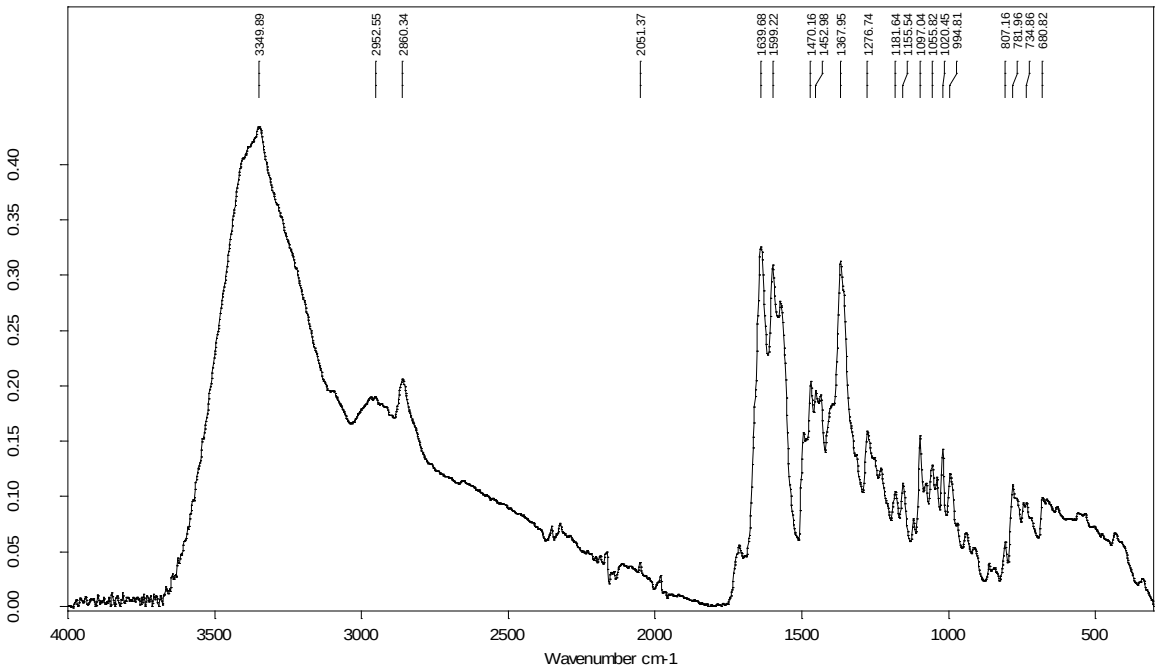
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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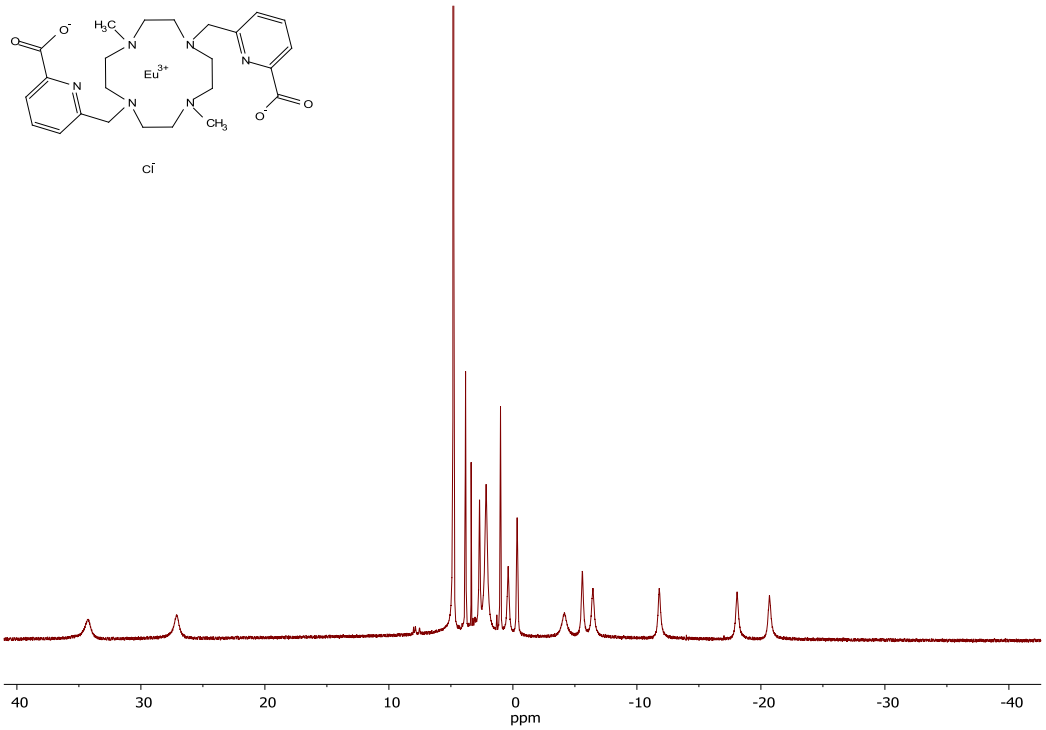
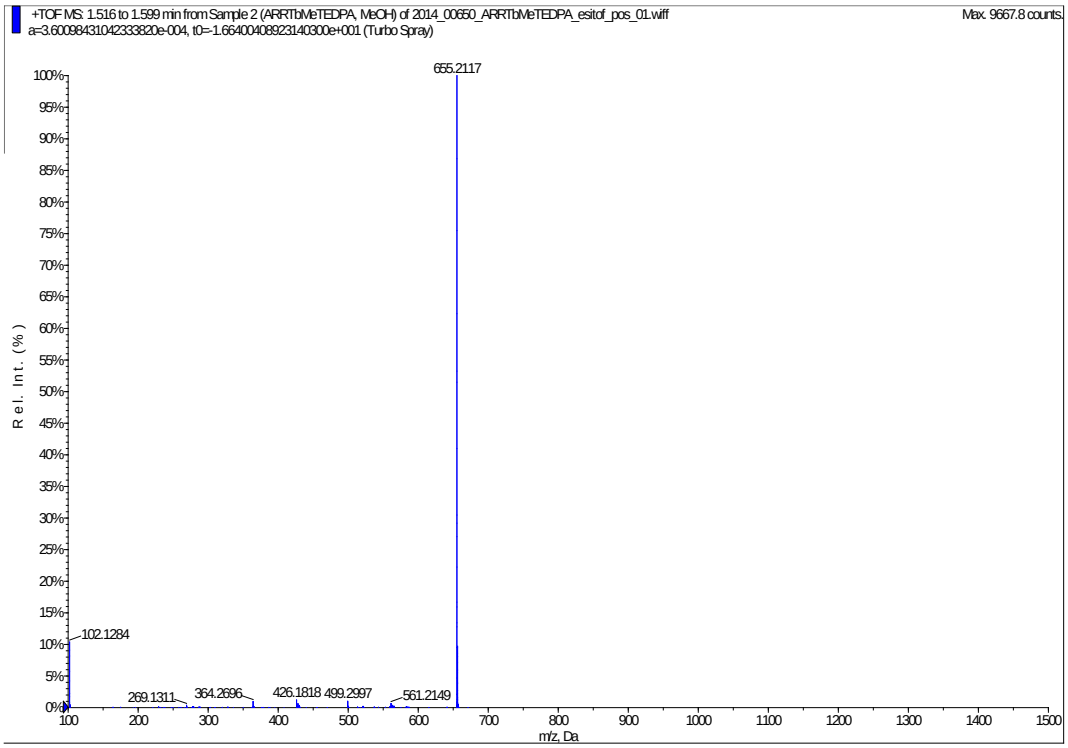
1276.74
1181.64
1155.54
1097.04
1055.82
1020.45
994.81
807.16
781.96
734.86
680.82
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(cb-tedpa)]Cl

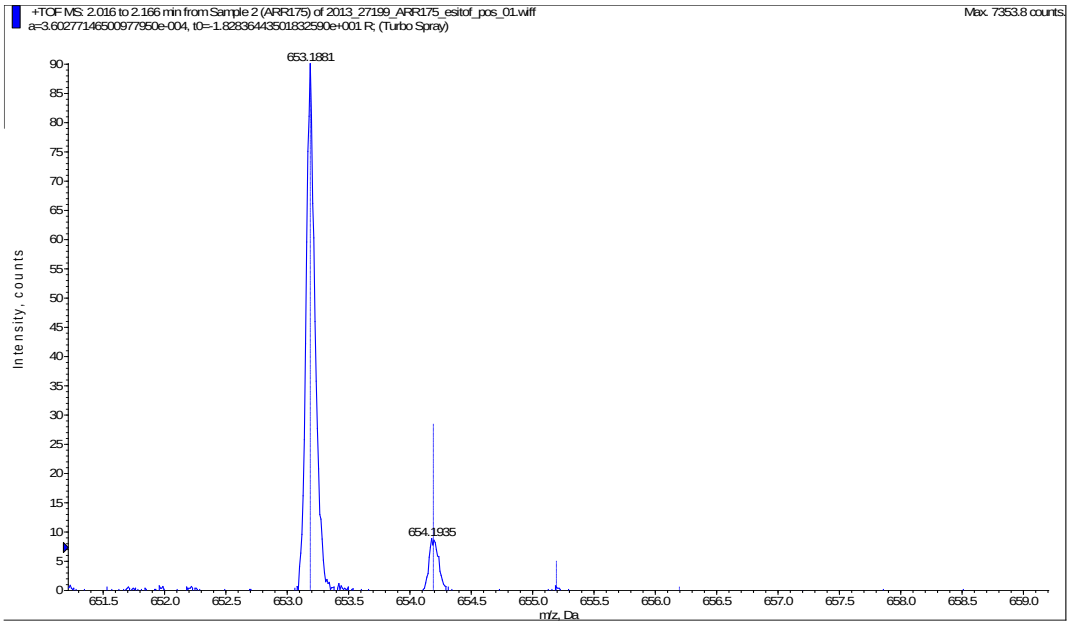
^{1}H-RMN (D_2O, 300 MHz) (δ/ppm)



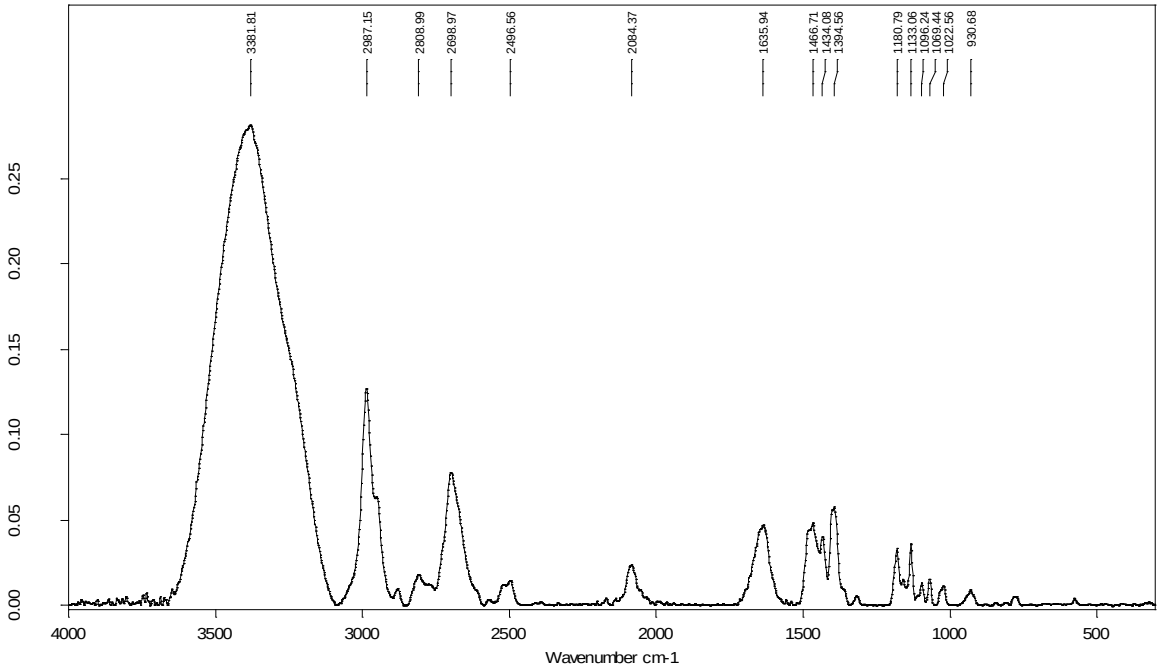
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

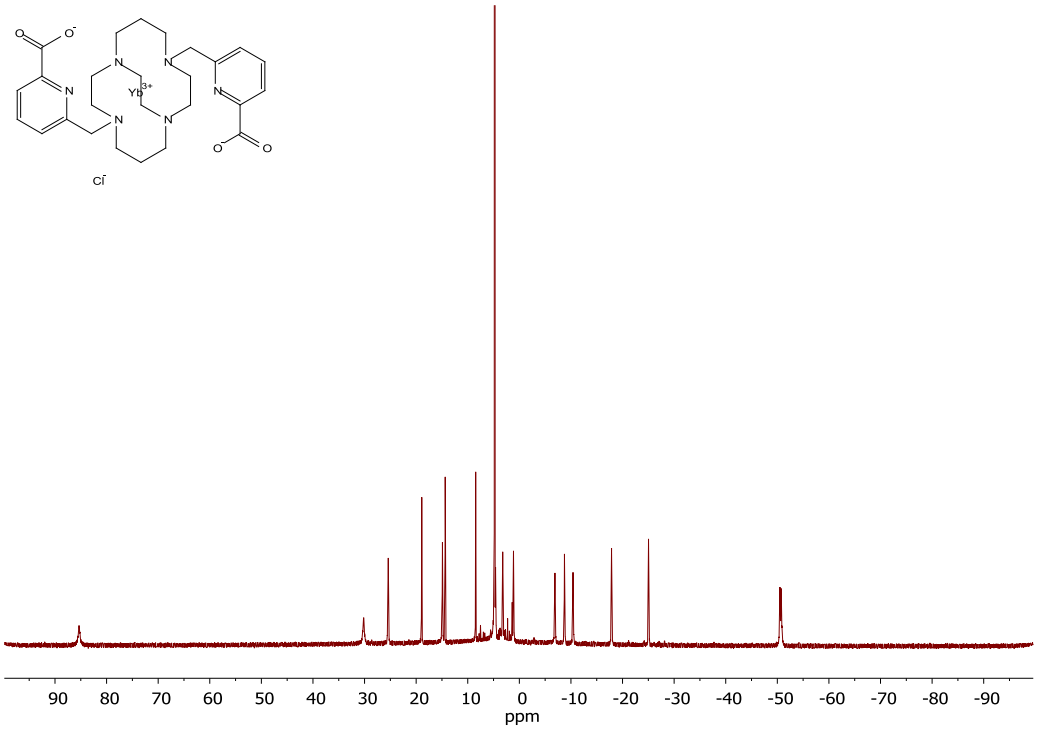


Espectro IR

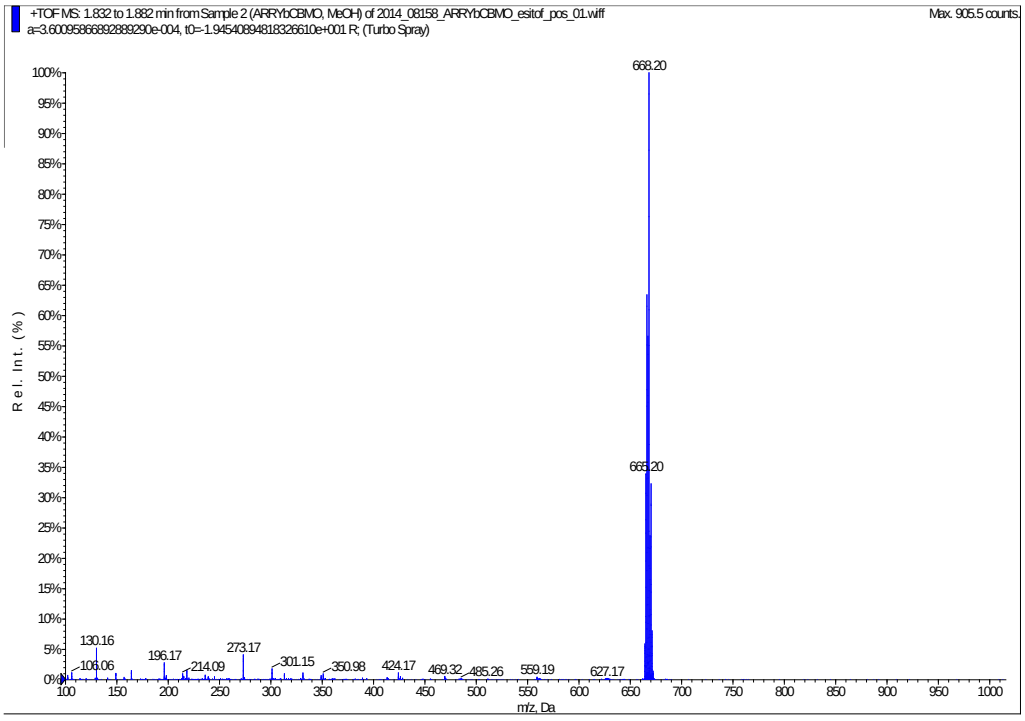


[Yb(cb-tedpa)]Cl

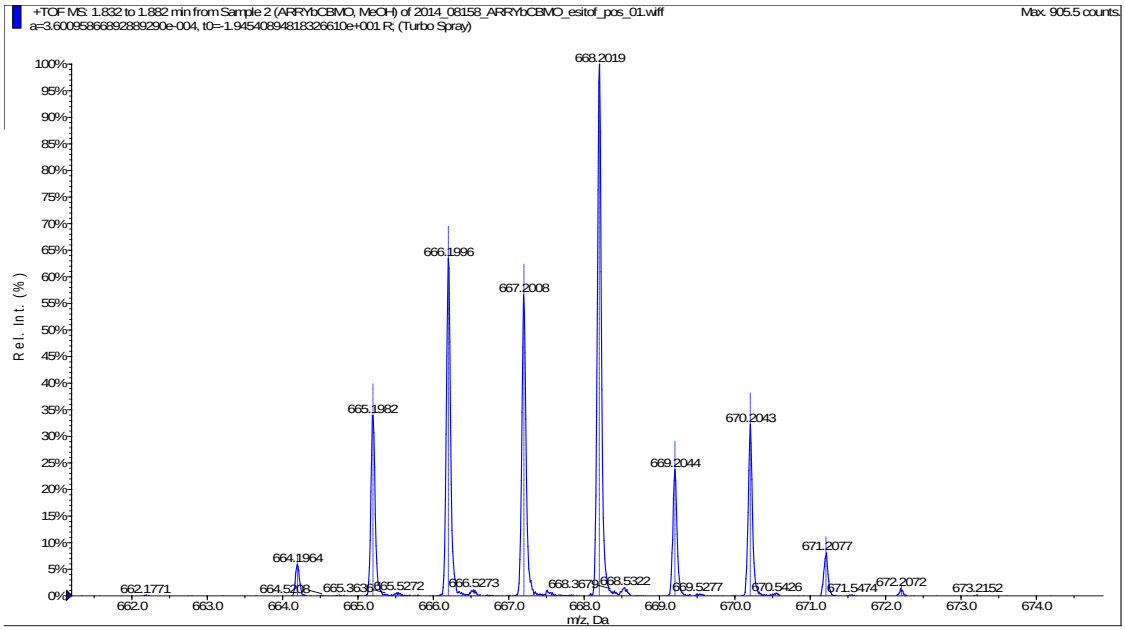
^{1}H-RMN (D_2O, 278K, 300 MHz) (δ/ppm)



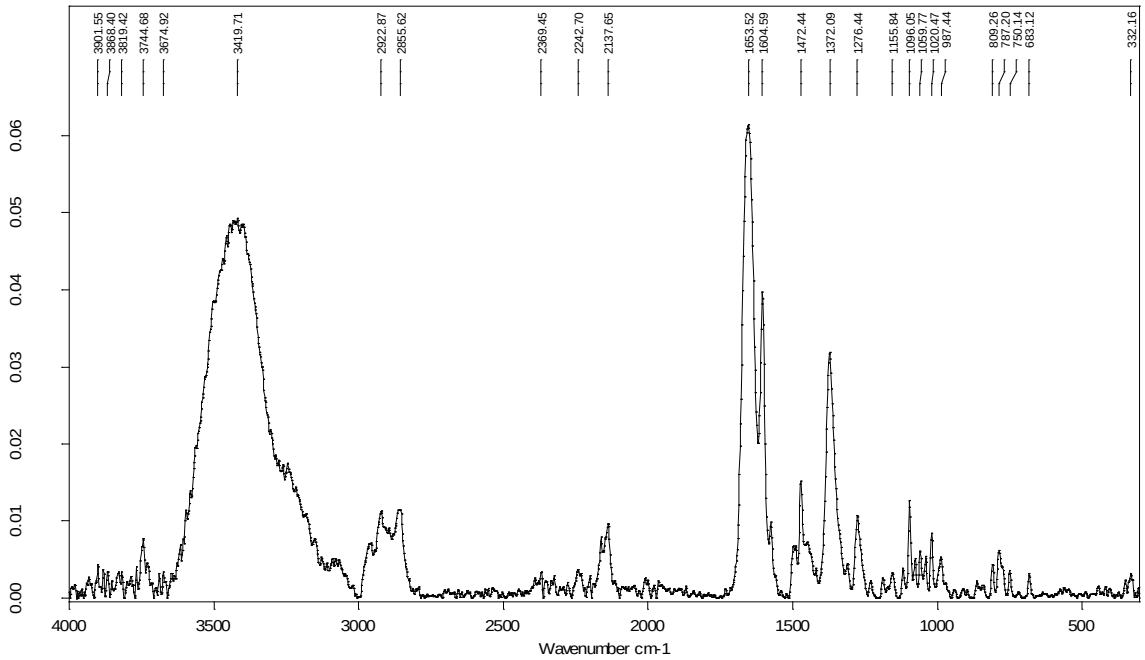
Espectro de masas ESI$^+$



Espectro ESI⁺ HR

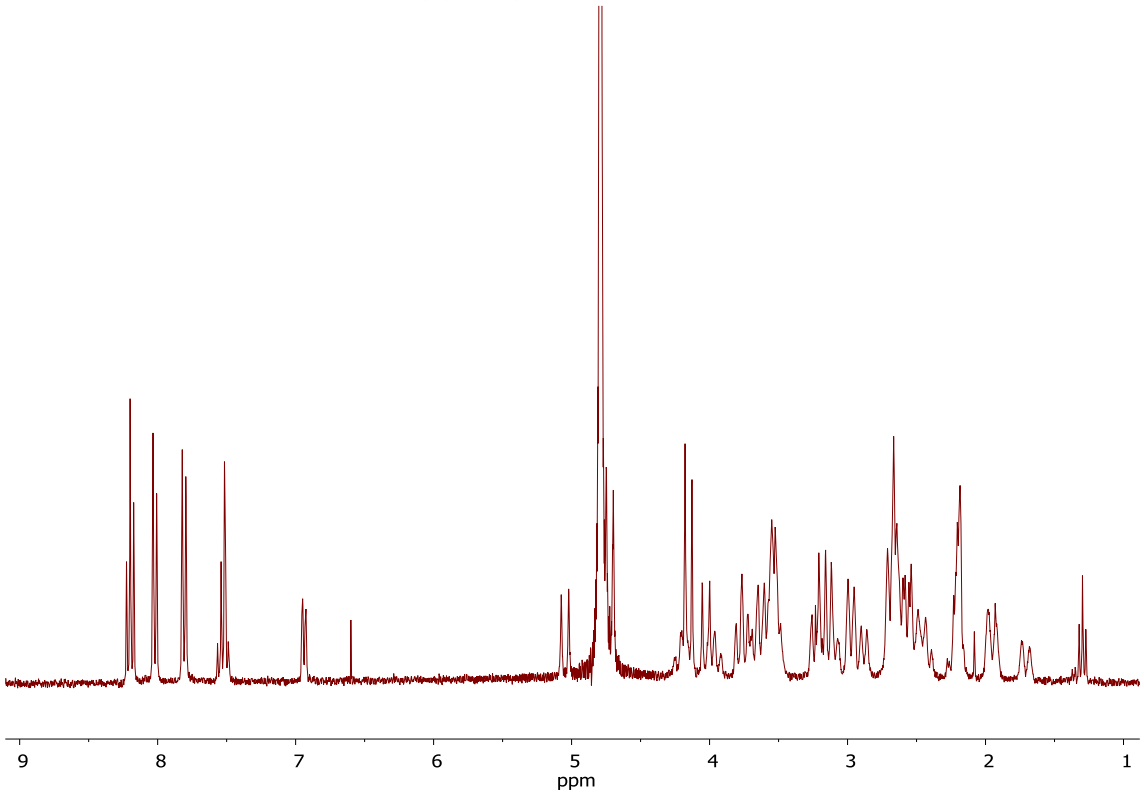


Espectro IR



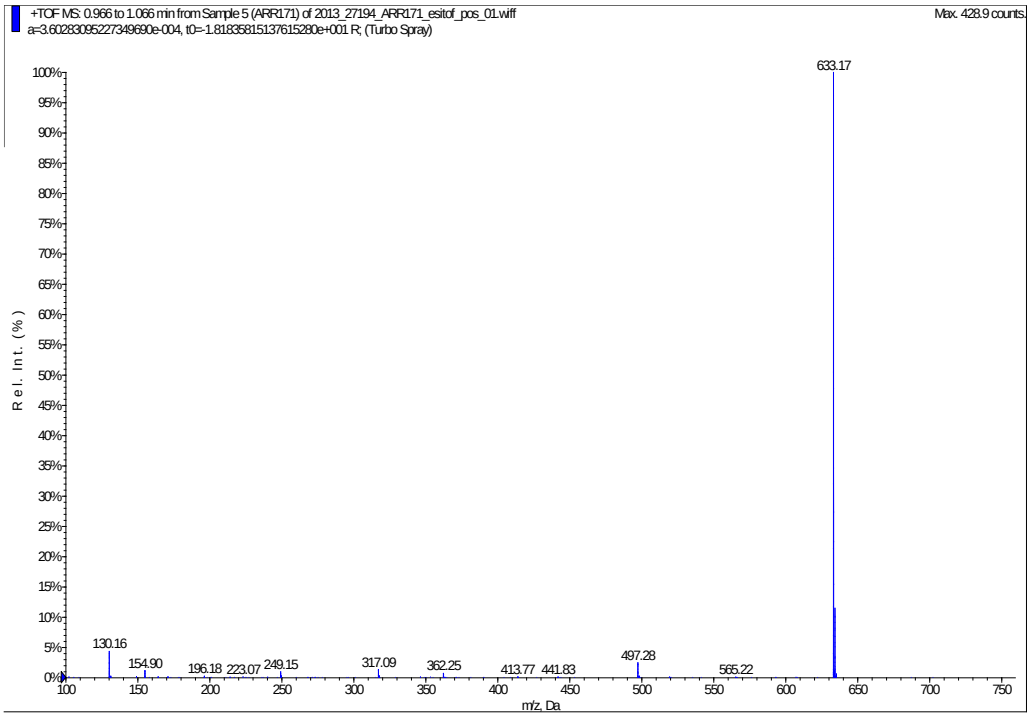
[La(cb-tedpa)]Cl (Complejo 2:1; $LaCl_3 \cdot 6H_2O$, EtOH 95 %, Et_3N)

^{1}H-RMN (D_2O, 500 MHz) (δ/ppm) pD = 5,89

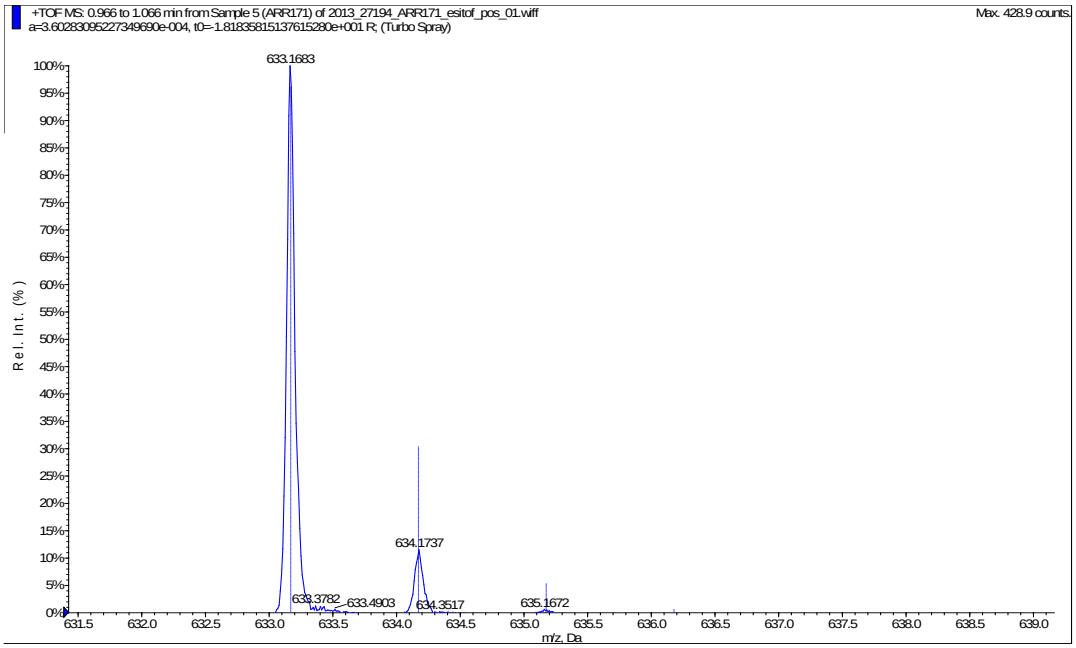


[La(cb-tedpa)](OTf)

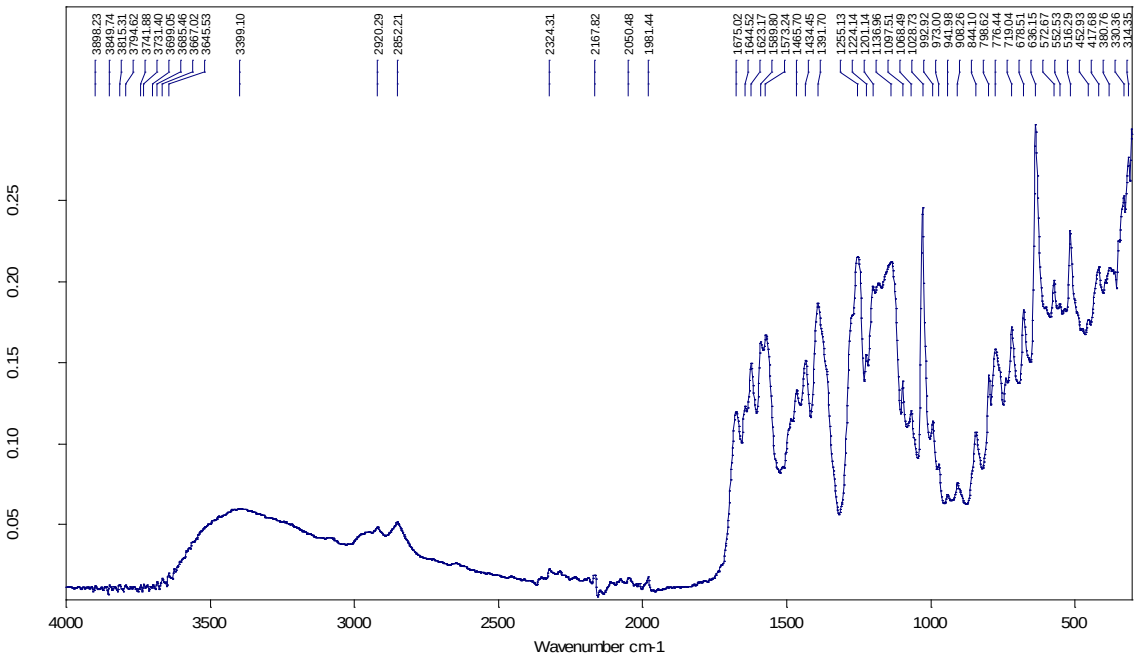
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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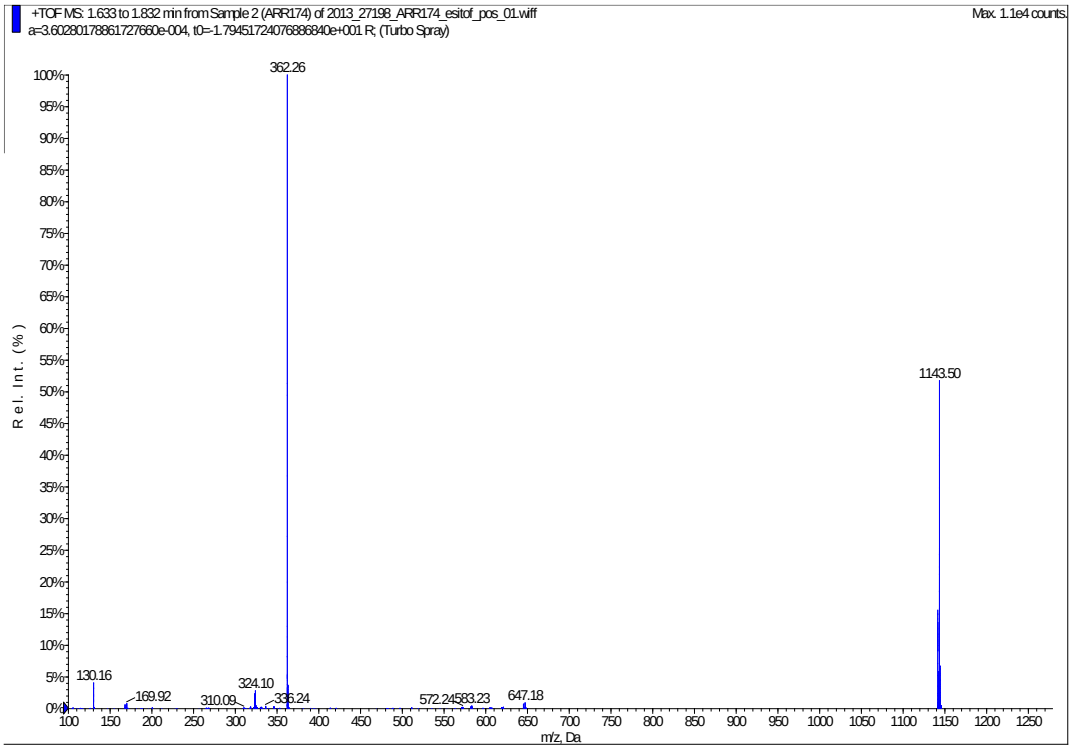
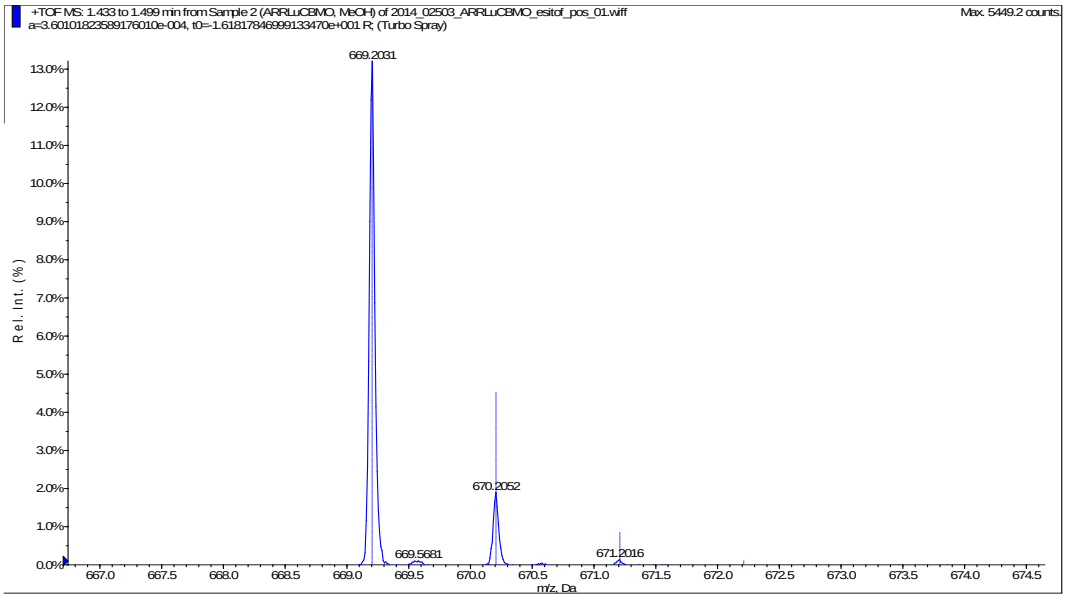
3815.31
3784.62
3741.88
3731.40
3699.05
3685.46
3667.02
3645.53
3399.10
2920.29
2852.21
2324.31
2167.82
2050.48
1981.44
1675.02
1644.52
1623.17
1589.80
1573.24
1465.70
1434.45
1391.70
1255.13
1224.14
1201.14
1158.96
1107.51
1068.49
1028.73
992.92
973.00
941.98
909.26
844.10
798.62
776.44
719.04
678.51
636.15
572.67
537.53
516.29
452.93
417.68
380.76
330.36
314.35
0.25
0.20
0.15
0.10
0.05
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Eu(cb-tedpa)](OTf)

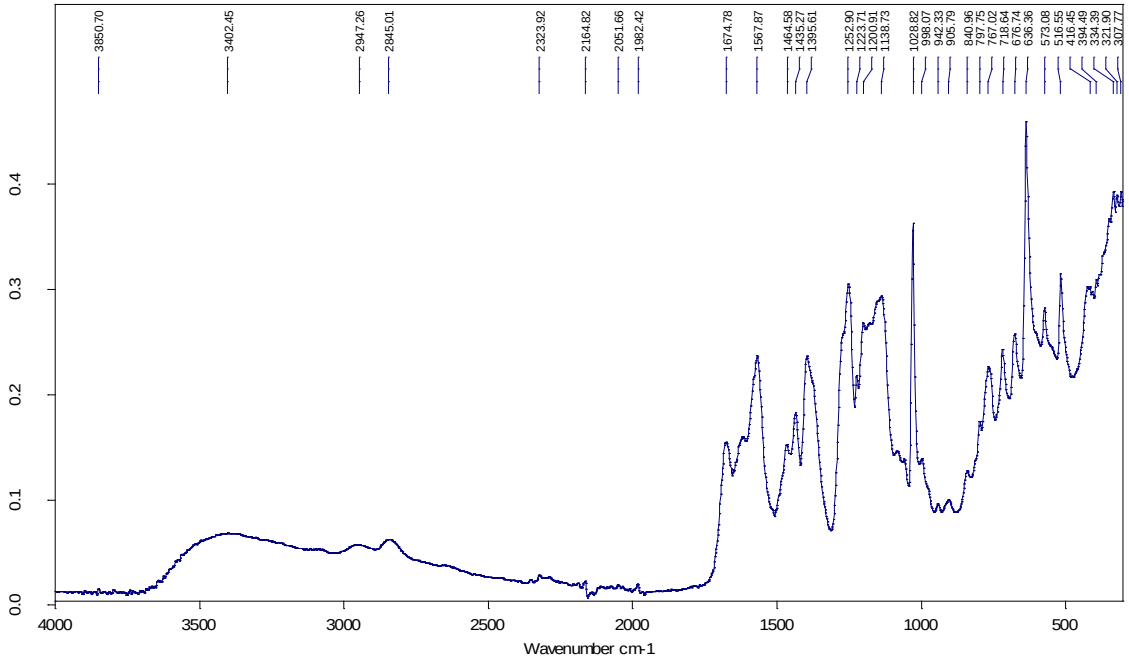
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR


3850.70
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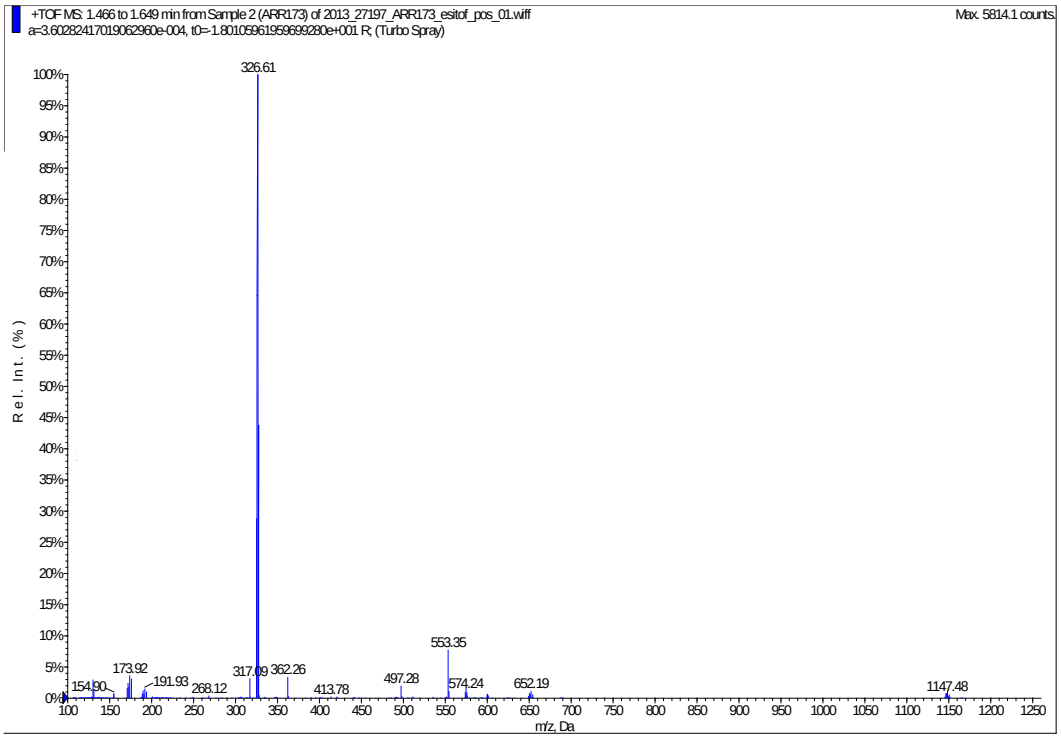
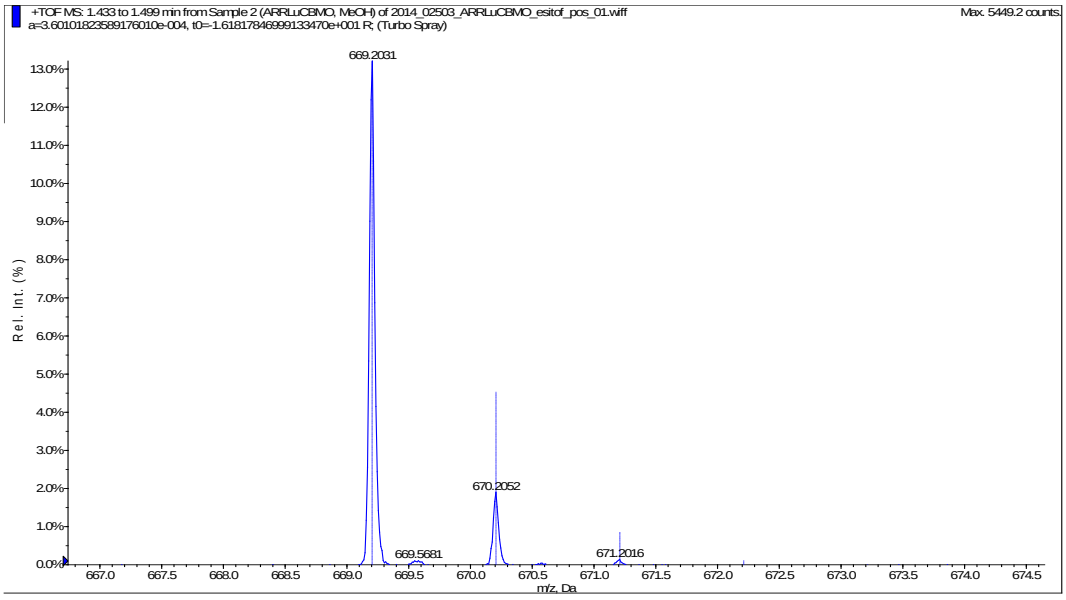
2947.26
2845.01
2323.92
2164.82
2051.66
1982.42
1674.78
1567.87
1464.58
1435.27
1395.61
1252.90
1223.71
1200.91
1138.73
1028.82
998.07
942.33
905.79
840.96
797.75
767.02
718.64
676.74
636.36
573.08
516.55
416.45
394.49
374.39
321.90
307.77
0.0
0.1
0.2
0.3
0.4
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Gd(cb-tedpa)](OTf)

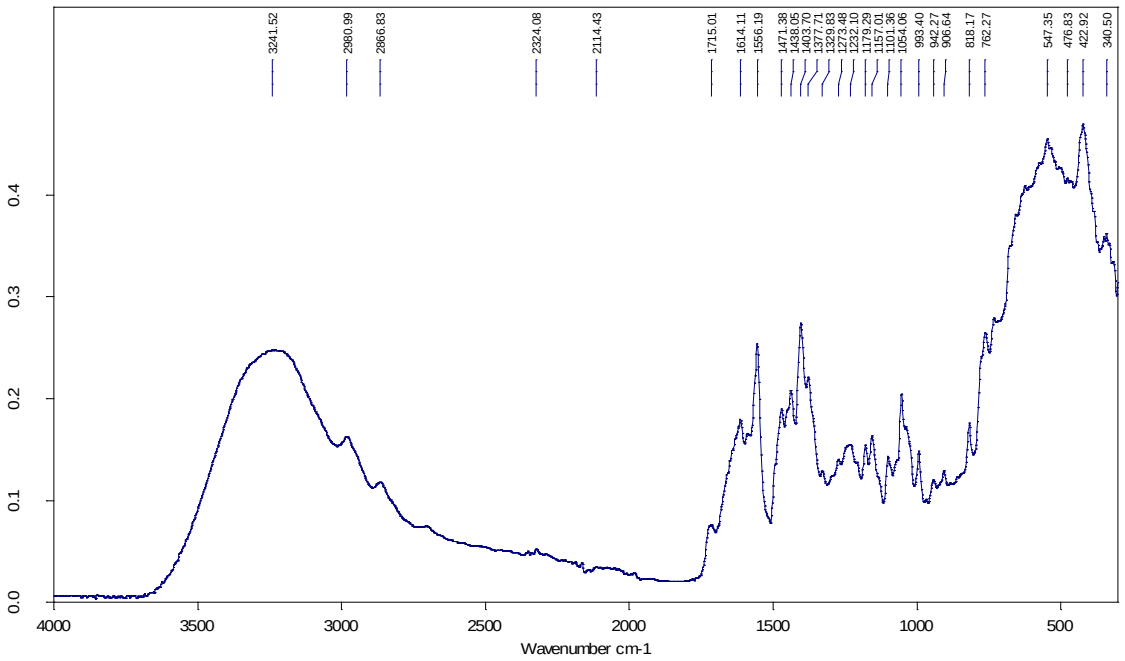
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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2866.83
2324.08
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1715.01
1614.11
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1471.38
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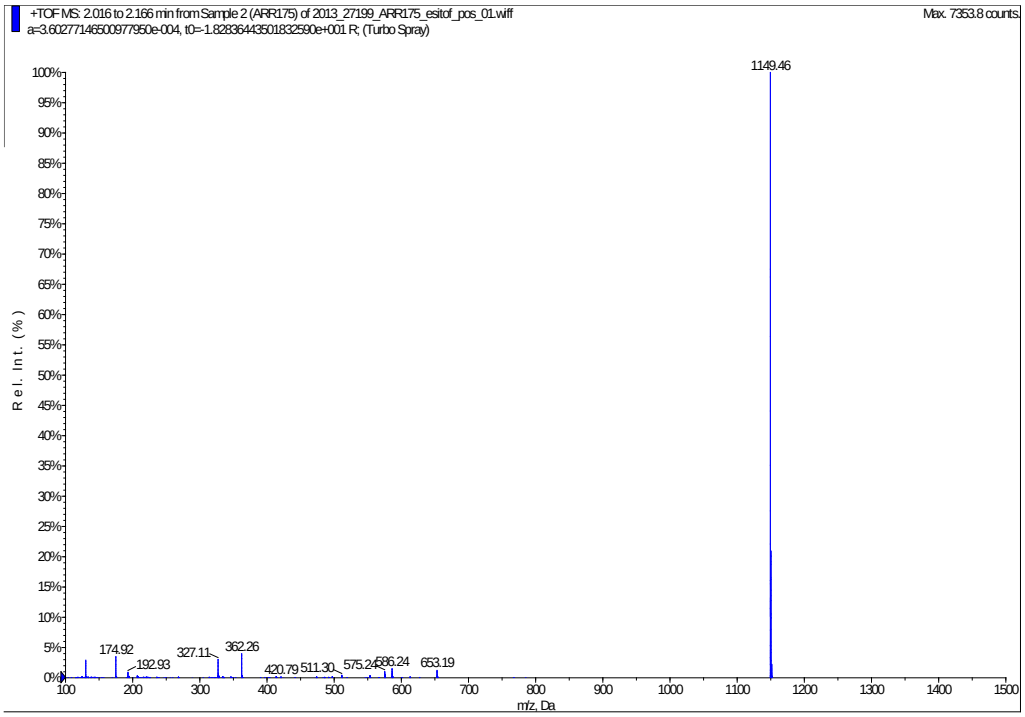
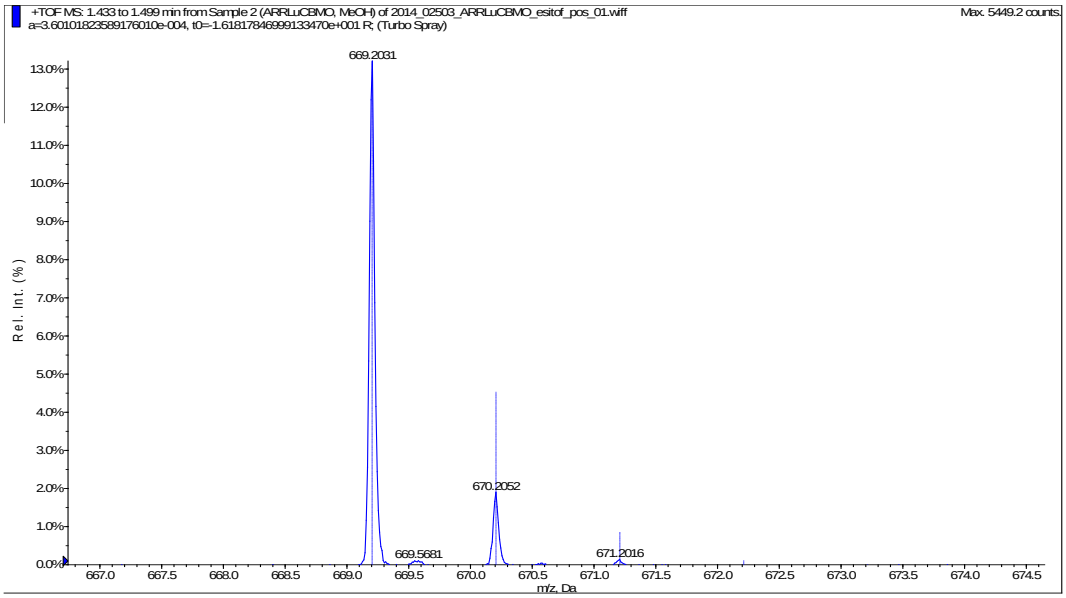
1403.70
1377.71
1329.83
1273.48
1232.10
1179.29
1157.01
1107.36
1054.06
993.40
942.27
906.64
818.17
762.27
547.35
476.83
422.92
340.50
0.0
0.1
0.2
0.3
0.4
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Tb(cb-tedpa)](OTf)

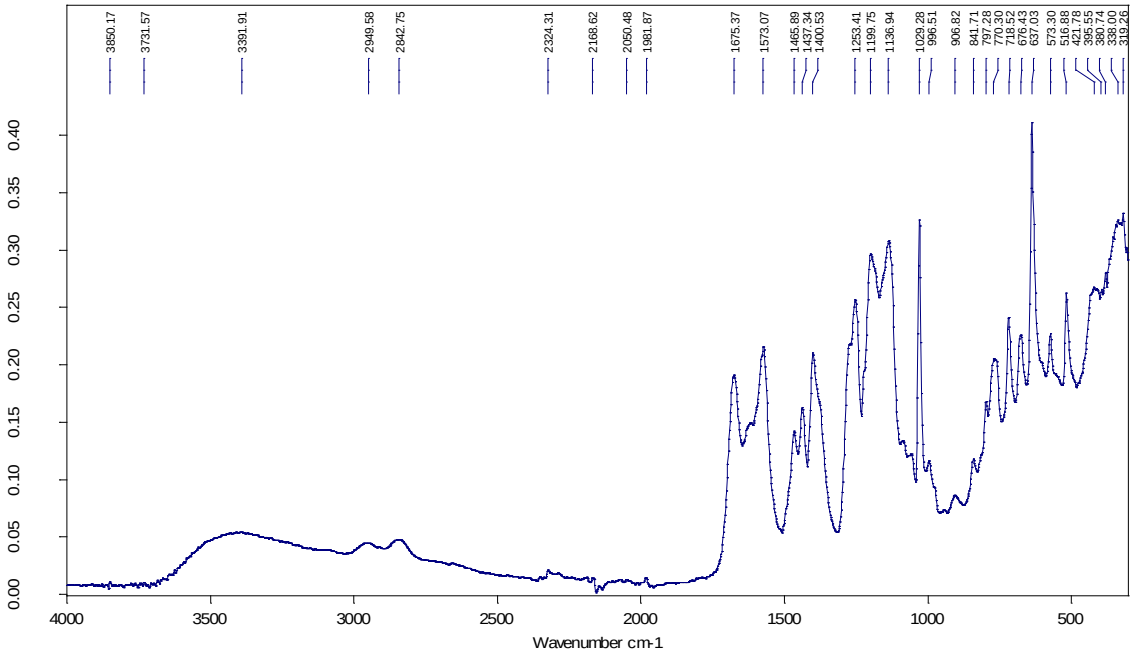
Espectro de masas ESI+



Espectro ESI+ HR

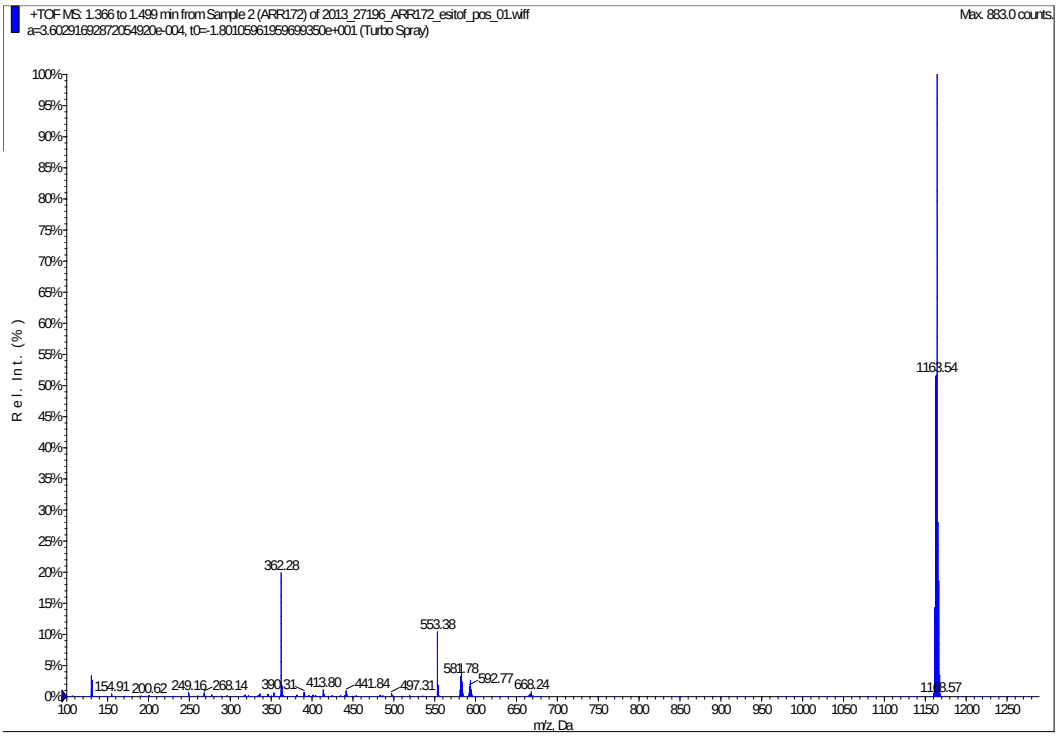


Espectro IR

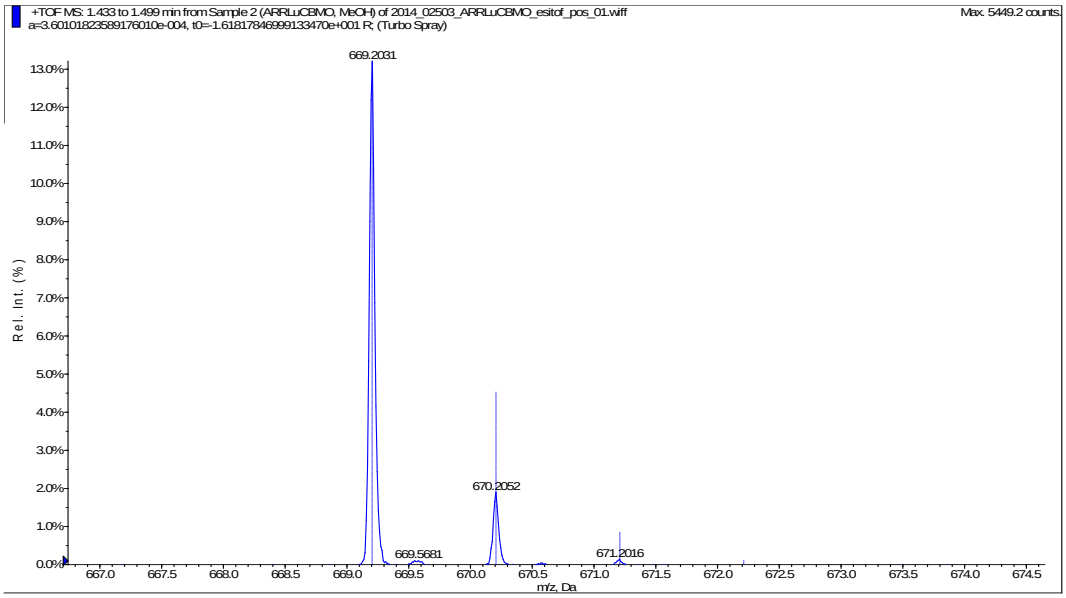

3850.17
3731.57
3391.91
2949.58
2842.75
2324.31
2168.62
2050.48
1981.87
1675.37
1573.07
1465.89
1437.34
1400.53
1253.41
1199.75
1136.94
1029.28
996.51
906.82
841.71
797.28
770.30
718.52
676.43
637.03
573.30
516.88
421.78
395.55
367.74
338.00
319.26
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Yb(cb-tedpa)](OTf)

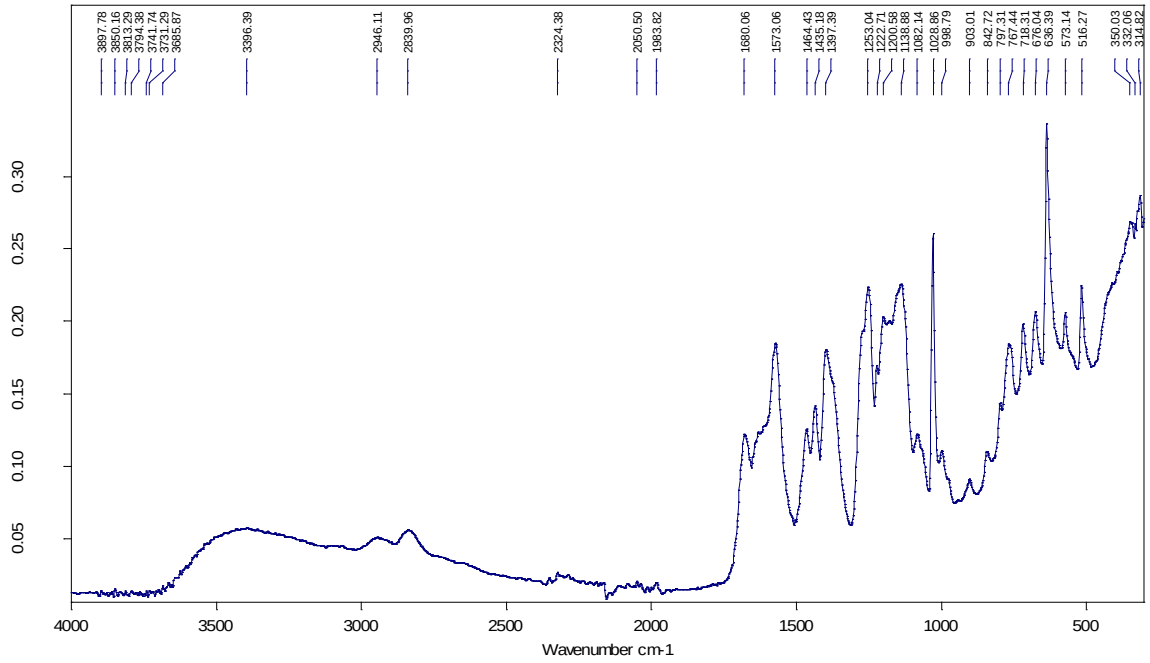
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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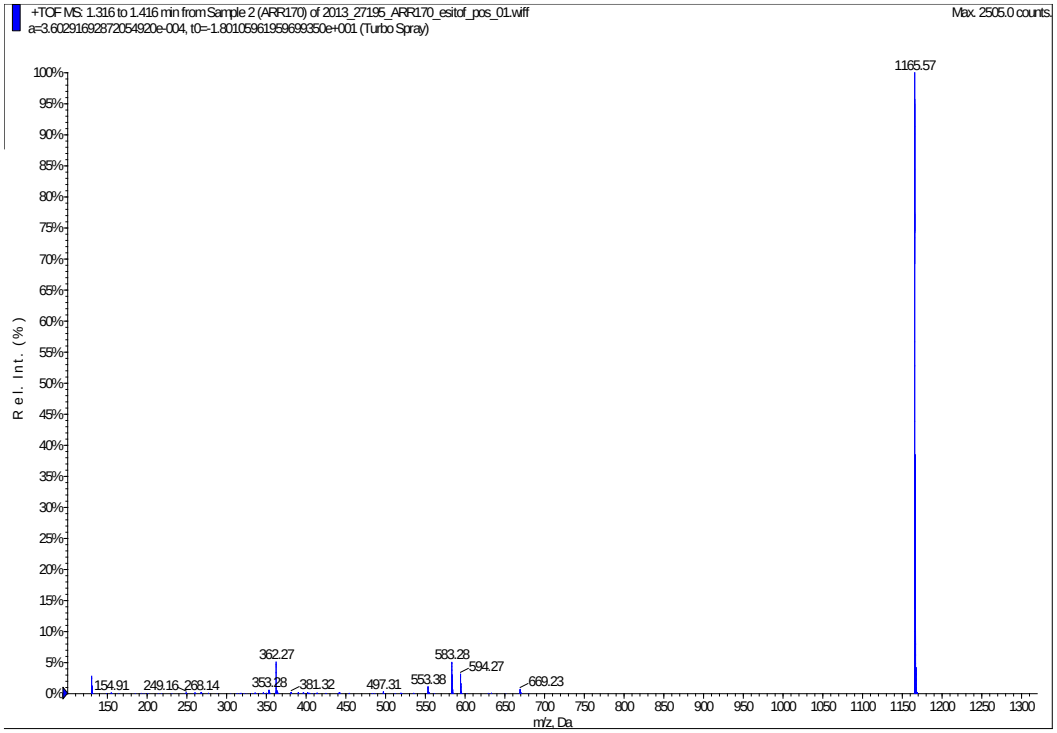
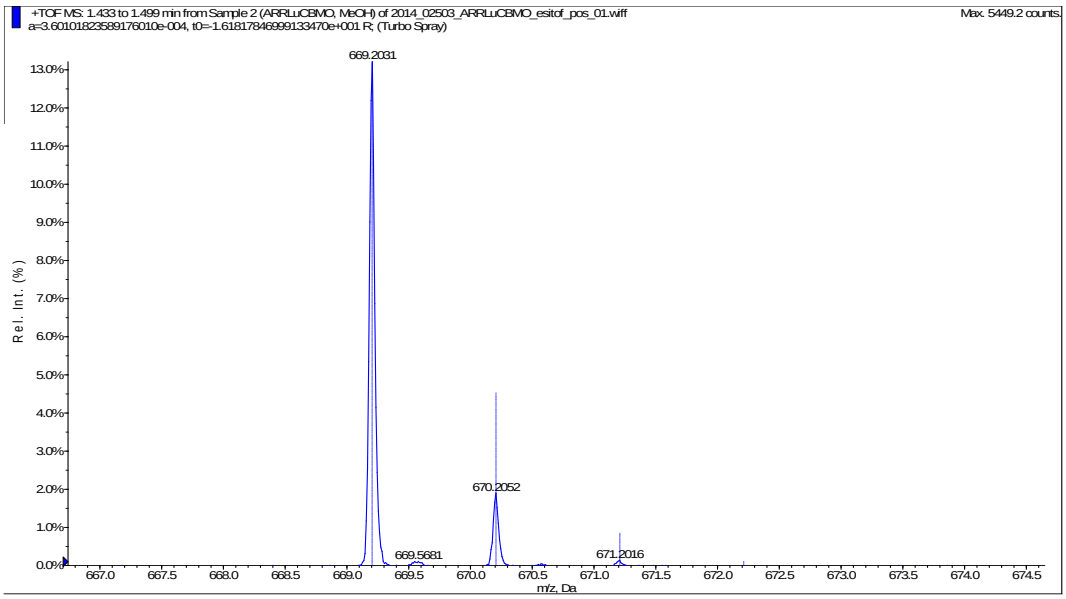
2324.38
2050.50
1983.82
1680.06
1573.06
1464.43
1435.18
1397.39
1253.04
1222.71
1200.58
1138.88
1082.14
1028.86
998.79
903.01
842.72
797.31
767.44
718.31
676.04
636.39
573.14
516.27
350.03
332.06
314.82
0.05
0.10
0.15
0.20
0.25
0.30
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

[Lu(cb-tedpa)](OTf)

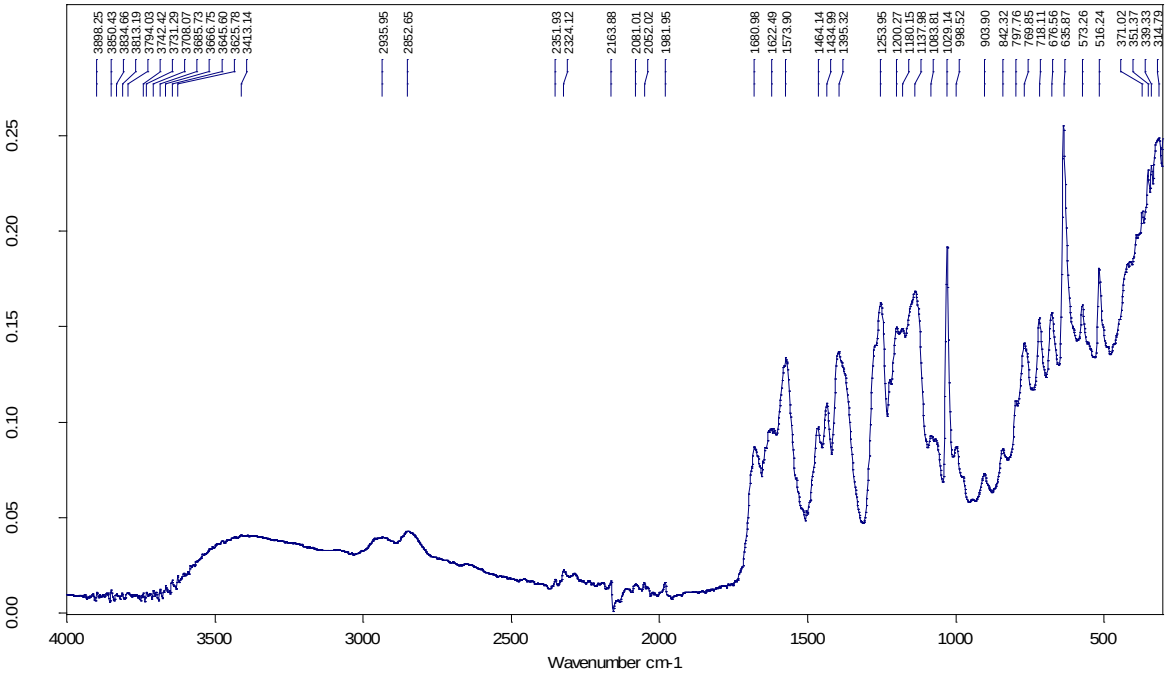
Espectro de masas ESI+



Espectro ESI+ HR



Espectro IR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3850.43
3834.66
3813.19
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3645.60
3625.78
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2935.95
2852.65
2351.93
2324.12
2163.88
2081.01
2052.02
1981.95
1680.98
1622.49
1573.90
1464.14
1434.99
1395.32
1253.95
1200.27
1180.15
1137.98
1083.81
1029.14
998.52
903.90
842.32
797.76
768.85
718.11
676.56
635.87
573.26
516.24
371.02
351.37
339.33
314.79
0.00
0.05
0.10
0.15
0.20
0.25
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

Química Computacional

MÉTODOS COMPUTACIONALES

La Química Computacional es uno de los modelos más avanzados que se han desarrollado hasta la fecha y una herramienta imprescindible para el estudio estructural de moléculas. Algunos métodos se pueden usar para modelar no solamente moléculas estables, sino también intermedios inestables de tiempos de vida cortos e incluso estados de transición. De esta forma, puede obtenerse información sobre moléculas y reacciones a la que no se tendría acceso con la simple observación. La gran importancia de los métodos teóricos en Química se ha reconocido a través de la concesión del Premio Nobel de Química en 1998 a Walter Kohn y a John A. Pople. Kohn desarrolló la "Teoría del Funcional de Densidad", mientras que Pople fue galardonado por el desarrollo de "Métodos Computacionales en Química Cuántica". En concreto, Pople diseñó programas informáticos basados en la Teoría Cuántica Clásica y en la Teoría del Funcional de Densidad.

Existen dos grandes áreas dentro de la Química Computacional dedicadas al estudio estructural de las moléculas y su reactividad: la Mecánica Molecular y la Teoría de la Estructura Electrónica. En ambas se realizan el mismo tipo básico de cálculos:

- Cálculo de la energía (y de otros parámetros relacionados) de una estructura molecular en particular.
- Optimización de geometrías que localicen la estructura molecular de más baja energía, próxima a la geometría de partida.
- Cálculo de frecuencias vibracionales de las moléculas, debidas a interacciones intramoleculares, que dependen de la segunda derivada de la función con respecto a las coordenadas atómicas.

Mecánica Molecular

Las simulaciones de Mecánica Molecular emplean las leyes de la Física Clásica para predecir las estructuras y propiedades moleculares. Existen diferentes métodos de Mecánica Molecular caracterizados por su particular *campo de fuerzas*. Un campo de fuerzas se compone de:

- Un conjunto de ecuaciones que definen cómo varía la energía potencial de una molécula con la posición de los átomos que la constituyen.
- Una serie de *átomos tipo* que definen las características de un elemento dentro de un contexto químico específico. Por ejemplo, un átomo de carbono en un grupo carbonilo se trata de forma diferente que uno enlazado a tres átomos de hidrógeno.
- Uno o más conjuntos de parámetros que ajustan las ecuaciones y los átomos tipo a los datos experimentales. Estos parámetros definen constantes de fuerza, que son valores usados en las ecuaciones para relacionar características atómicas con la energía y datos estructurales como distancias y ángulos de enlace.

Los cálculos de Mecánica Molecular no tratan explícitamente los electrones de un sistema molecular, sino que basan sus cálculos en interacciones entre núcleos. Los efectos electrónicos se incluyen en los campos de fuerza. Esta aproximación hace que los cálculos de Mecánica Molecular sean poco costosos desde el punto de vista computacional, de manera que pueden aplicarse a sistemas con muchos miles de átomos. Sin embargo, la Mecánica Molecular presenta una serie de limitaciones:

- Cada campo de fuerzas proporciona buenos resultados para un número limitado de moléculas relacionadas con aquellas con las que ha sido parametrizado.
- Dado que los efectos electrónicos se incluyen de forma implícita en el campo de fuerza mediante parametrización, los métodos de Mecánica Molecular no pueden tratar problemas químicos donde predominan los efectos electrónicos, como por ejemplo procesos que involucren la formación o ruptura de enlaces.

Métodos de Estructura Electrónica

Los métodos de Estructura Electrónica utilizan las leyes de la Mecánica Cuántica en vez de las de la Física Clásica, como base para sus cálculos. La Química Cuántica afirma que la energía, así como otras propiedades de la molécula, pueden obtenerse mediante la resolución de la ecuación de Schrödinger ($H\cdot\psi = E\cdot\psi$ Ecuación 1):

$$H\cdot\psi = E\cdot\psi \qquad \text{Ecuación 1}$$

Sin embargo, salvo para los sistemas más pequeños, no es posible resolver esta ecuación de forma exacta, caracterizándose los métodos de Estructura Electrónica por las diferentes aproximaciones matemáticas a la solución. Las distintas clases de métodos de Estructura Electrónica son:

- Los *Métodos Semi-Empíricos*, que usan parámetros derivados de datos experimentales con el fin de simplificar los cálculos. De este modo, la resolución aproximada de la ecuación de Schrödinger depende de la disponibilidad de parámetros adecuados para el tipo de sistema químico que se quiera estudiar.
- Los *Métodos Ab Initio*, que no utilizan parámetros experimentales en sus cálculos, sino que se basan en las leyes de la Mecánica Cuántica y en un pequeño número de constantes físicas como son: la velocidad de la luz, las masas y cargas de los electrones y núcleos y la constante de Planck.
- Los *Métodos de Funcional de Densidad* (*DFT*), que son similares a los Métodos Ab Initio más sencillos, pero incluyen los efectos de la correlación electrónica.

Modelos Químicos

Un modelo teórico debe ser uniformemente aplicable a sistemas moleculares de cualquier tamaño y tipo, hasta un tamaño máximo que viene determinado únicamente por la disponibilidad práctica

de fuentes computacionales. Por tanto, un modelo teórico debe estar especialmente definido para cualquier configuración de núcleos y electrones. Esto significa que lo único que se requiere para obtener una solución aproximada de la ecuación de Schrödinger es especificar la estructura molecular. No se necesita ningún otro parámetro para especificar el problema o su solución. Por otra parte, un modelo teórico debe ser imparcial, no debe confiar en suposiciones previas sobre la estructura molecular o los procesos químicos, pues éstas lo harían inadecuado para ciertas clases de sistemas o fenómenos en los que dichas suposiciones no se pudiesen aplicar. En general, no se debe recurrir a procedimientos especiales para tipos específicos de moléculas.

Una vez que un modelo teórico ha sido definido y ejecutado, debe ser examinado sistemáticamente sobre diferentes sistemas químicos y sus resultados deben ser comparados con los valores experimentales conocidos. Tras demostrarse que el modelo puede reproducir los resultados experimentales, se puede utilizar para predecir las propiedades de aquellos sistemas para los que no se dispone de datos experimentales.

Un modelo químico está caracterizado por la combinación de un procedimiento teórico y un conjunto base, que consiste en una representación matemática de los orbitales moleculares de la molécula. Los modelos teóricos más utilizados se recogen en la Tabla 1. Hay que tener en cuenta que cuanto más exacto es el método teórico utilizado, mayor es su coste computacional.

Tabla 1. Métodos teóricos más comunes.

Método	Descripción
HF	Teoría del campo autoconsistente de Hartree-Fock
DFT	Teoría del funcional de densidad
MP2	Teoría de la perturbación de segundo orden de Møller-Plesset
MP4 (SDQ)	Teoría de la perturbación de cuarto orden de Møller-Plesset, sin las contribuciones triples
QCISD	Interacción de configuración cuadrática
CCSD	coupled cluster singles doubles
CID	Interacción de configuración con excitaciones dobles
CISD	Interacción de configuración con excitaciones sencillas y dobles

Conjunto Base

Un conjunto base es una descripción matemática de los orbitales de un sistema molecular; se trata de una aproximación que consiste en representar los orbitales moleculares como combinaciones lineales de un conjunto predefinido de funciones monoelectrónicas de tipo gausiano conocidas como *funciones base*. Los conjuntos base más grandes constituyen una aproximación más exacta de los orbitales, pues imponen pocas restricciones sobre la localización de los electrones en el espacio. Las

funciones base están normalmente centradas en el núcleo atómico y tienen algún parecido con los orbitales atómicos. Sin embargo, el tratamiento matemático actual es más general, y se puede utilizar cualquier conjunto de funciones, siempre y cuando se definan de forma apropiada. Un orbital molecular individual se define como:

$$\boldsymbol{\varphi}_i = \sum_{\boldsymbol{\mu}=1}^{N} c_{\boldsymbol{\mu}i}\ \boldsymbol{\chi}_{\boldsymbol{\mu}} \qquad \text{Ecuación 2}$$

donde $c_{\mu i}$ son los coeficientes de expansión del orbital molecular y las funciones base χ_μ se eligen normalizadas. Se emplea el convenio de notación que utiliza caracteres latinos para las funciones de los orbitales moleculares y caracteres griegos para las funciones base. Por lo tanto, χ_μ se refiere a una función base arbitraria de la misma forma que φ_i se refiere a un orbital molecular arbitrario. *Gaussian* y otros programas *Ab Initio* de estructura electrónica utilizan funciones atómicas de tipo gausiano como funciones base. Una función gausiana tiene la fórmula general:

$$g(\boldsymbol{\alpha}, \vec{r}) = c\, x^n\, y^m\, z^l\, e^{-\boldsymbol{\alpha} r^2} \qquad \text{Ecuación 3}$$

donde α es una constante que determina el tamaño (extensión radial) de la función. En la función gausiana, el término $e^{-\alpha r^2}$ es multiplicado por potencias de x, y, z, y una constante de normalización, de tal manera que la integral en todo el espacio sea la unidad:

$$\int_{\text{espacio}} g^2 = 1 \qquad \text{Ecuación 4}$$

Por tanto, la constante c depende tanto del valor de α como de los valores de n, m y l. En la ecuación anterior, x, y y z son las coordenadas electrónicas cartesianas y n, m y l son conjuntos de números enteros mayores o iguales a cero. Estos números no pueden asociarse a los números cuánticos, aunque caracterizan la simetría de las funciones de base (Tabla 2).

Tabla 2. Valores de n, m y l y su relación con la simetría.

n	m	l	n + m+ l	Simetría
0	0	0	0	s
1	0	1	1	p_x
0	1	0	1	p_y
0	0	1	1	p_z
2	0	0	2	d_{x^2}
0	2	0	2	d_{y^2}
0	0	2	2	d_{z^2}
1	1	0	2	d_{xy}
1	0	1	2	d_{xz}
0	1	1	2	d_{yz}

Puede verificarse que la suma de n + m + l produce los números cuánticos de momento angular que caracterizan las funciones del tipo *s*, *p*, *d*... A continuación se muestran algunas funciones gausianas representativas de las funciones tipo s, p_y y d_{xy}:

$$g_s(\boldsymbol{\alpha},\vec{r}) = \left(\frac{2\boldsymbol{\alpha}}{\boldsymbol{\pi}}\right)^{3/4} e^{-\alpha r^2} \qquad \text{Ecuación 5}$$

$$g_{p_y}(\boldsymbol{\alpha},\vec{r}) = \left(\frac{\mathbf{128}\boldsymbol{\alpha}^5}{\boldsymbol{\pi}^3}\right)^{1/4} y\, e^{-\alpha r^2} \qquad \text{Ecuación 6}$$

$$g_{d_{xy}}(\boldsymbol{\alpha},\vec{r}) = \left(\frac{\mathbf{2048}\boldsymbol{\alpha}^7}{\boldsymbol{\pi}^3}\right)^{1/4} x\, y\, e^{-\alpha r^2} \qquad \text{Ecuación 7}$$

Se utilizan combinaciones lineales de funciones gausianas de este tipo para formar las funciones base, denominándose éstas gausianas contraídas, que tienen la forma:

$$\boldsymbol{\chi}_{\boldsymbol{\mu}} = \sum_p d_{\mu p} g_p \qquad \text{Ecuación 8}$$

donde $d_{\mu p}$ es el coeficiente de contracción (se trata de una constante fija para un conjunto base dado) y p es el número de funciones gausianas primitivas que componen la función base. Una función base compuesta de una única gausiana se denomina no-contraída. Todas estas consideraciones llevan a la siguiente expresión para los orbitales moleculares:

$$\boldsymbol{\phi}_i = \sum_{\boldsymbol{\mu}} c_{\mu i}\, \boldsymbol{\chi}_{\boldsymbol{\mu}} = \sum_{\boldsymbol{\mu}} c_{\mu i} \left(\sum_p d_{\mu p}\, g_p\right) \qquad \text{Ecuación 9}$$

Los ***conjuntos base mínimos*** contienen el número mínimo de funciones base que se necesitan para cada átomo. Este conjunto sólo incluye los orbitales internos y de valencia. Por ejemplo, un conjunto base mínimo describe los átomos de H o C de la siguiente manera:

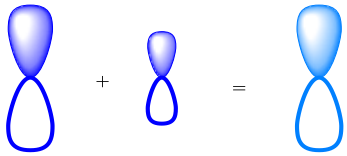
- H: 1*s*
- C: 1*s*, 2*s*, 2p_x, 2p_y, 2p_z

Los conjuntos base mínimos utilizan orbitales de tipo atómico de tamaño fijo. Por ejemplo, el conjunto base STO-3G es un conjunto base mínimo (aunque no el conjunto base más pequeño posible). Utiliza tres funciones gausianas primitivas por función base, tal y como indica 3G en su nombre. STO significa orbitales de tipo Slater (*Slater-Type Orbitals*). Es decir, el conjunto base STO-3G aproxima los orbitales de Slater con tres funciones gausianas. De hecho, los orbitales de tipo Slater proporcionan más precisión en cálculos de orbitales moleculares que un número similar de funciones gausianas, pero son más difíciles de utilizar por cuestiones matemáticas.

Una primera manera con la que se puede hacer un conjunto base mayor es incrementar el número de funciones base por átomo (***conjuntos base extendidos***). En este caso, se tienen en cuenta los orbitales internos, los orbitales de valencia y, además, un conjunto de orbitales no ocupados llamados orbitales virtuales. Por ejemplo, para el átomo de carbono tendríamos los orbitales 1*s*, 2*s*, 2p_x, 2p_y, 2p_z,

3*s*, 3p_x, 3p_y, 3p_z. Entre los conjuntos base de tipo extendido, cabe destacar: los conjuntos base del tipo *split valence*, los conjuntos base polarizados y las funciones difusas.

Los **conjuntos base del tipo *split valence*** aumentan el tamaño de la base creando orbitales similares a los que se utilizan normalmente pero con tamaño diferente. Así, el átomo de carbono se describiría de la siguiente manera:

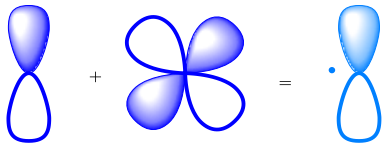


C_1 C_2

C: 1*s*, 2*s*´,2p_x, 2p_x´, 2p_y, 2p_y´,2p_z, 2p_z´

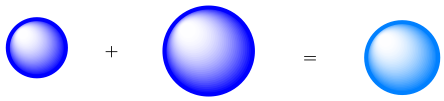
donde las funciones con o sin prima tienen la misma simetría pero difieren en el tamaño. Conjuntos base típicos del tipo *split valence* son el 3-21G y el 6-31G. Del mismo modo, los conjuntos base del tipo *triple split valence* utilizan tres funciones de diferente tamaño para cada tipo de orbital atómico.

Los ***conjuntos base polarizados*** añaden orbitales con un momento angular mayor que el requerido para la descripción de cada átomo. Por ejemplo, un conjunto base polarizado añade una función *d* a un carbono o una función *f* a un metal de transición y en algunos casos, añade una función *p* al átomo de hidrógeno. Los conjuntos base polarizados permiten, en cierta medida, cambiar la forma de los orbitales. Por ejemplo, el conjunto base 6-31G(d) (ó 6-31G*) añade una función *d* en átomos pesados. El conjunto base 6-31G(d, p) (ó 6-31G**) añade funciones *p* a los átomos de H además de funciones *d* a los átomos pesados:



C_1 C_2

Las ***funciones difusas*** son versiones de gran tamaño de funciones del tipo *s* y *p* que hacen que la función orbital decaiga de manera mucho más suave (añadiendo para ello contribuciones espaciales al orbital) y permiten a los orbitales ocupar una región más grande del espacio. Las funciones difusas son muy importantes para sistemas donde los electrones están relativamente lejos del núcleo como moléculas cargadas, sistemas en estado excitado, sistemas con bajos potenciales de ionización, descripción de la acidez absoluta, etc... El conjunto base 6-31+G(d) es idéntico al 6-31G(d), pero añadiendo funciones difusas en los átomos pesados. La versión 6-31++G(d) añade funciones difusas a los hidrógenos.



C_1 C_2

En el proceso de formación de moléculas y cristales, sólo los electrones de *valencia* juegan un papel relevante, mientras que los electrones más internos (los del *core*), se mantienen esencialmente igual que en los átomos separados. Esta es la base del desarrollo de métodos mecanocuánticos *ab initio* aproximados, en los que sólo se calculan explícitamente las funciones de onda y las energías de los electrones de valencia, eso sí, sometidos a la influencia de los electrones internos, además de a los núcleos o a otros campos externos. Los efectos de los electrones del *core* se incluyen por medio de los ***Potenciales Efectivos del Core***, recibiendo los métodos que tienen en cuenta esta interacción el nombre genérico de ECP (es decir, se trata de métodos que usan potenciales efectivos del *core* basados en la aproximación del *core congelado*). Los métodos ECP pueden agruparse en dos familias:

- la familia de los *Pseudopotenciales*: basada en la aceptación de la *transformación pseudoorbital*, y cuyo origen se encuentra en la ecuación de Phillips-Kleinman[62].
- la familia de los *Potenciales Modelo*: no realiza ninguna transformación orbital y se basa en la ecuación de Huzinaga-Cantu[63].

Hoy en día, los métodos ECP se usan ampliamente en cálculos *ab initio* de moléculas en disolución y en estructuras cristalinas. De hecho, en la inmensa mayoría de los cálculos *ab initio* con sistemas en los que está presente algún elemento pesado o semipesado se utilizan ECPs. La principal razón de su uso está en el ahorro de cálculo asociado, pues sólo se tratan los electrones de valencia, y la sencillez y eficacia con la que se incluyen los efectos relativistas más importantes en los cálculos moleculares con ECPs. Otra de las ventajas del uso de ECPs es que se elimina en gran medida el error de superposición del conjunto base (BSSE), que se debe primordialmente a deficiencias en la representación de los electrones más internos.

Métodos de Hartree-Fock (HF) y del Funcional de Densidad (DFT)

Tal y como se indicó en la sección anterior, un determinado orbital molecular viene dado por la siguiente expresión:

$$\boldsymbol{\phi}_i = \sum_{\mu} c_{\mu i}\, \boldsymbol{\chi}_{\mu} = \sum_{\mu} c_{\mu i} \left(\sum_p d_{\mu p}\, g_p \right) \qquad \text{Ecuación 10}$$

donde: g_p es una función gausiana primitiva, $d_{\mu p}$ son constantes fijas para un conjunto base determinado, $c_{\mu i}$ son los coeficientes de expansión del orbital molecular.

El problema que se plantea a continuación es como obtener este conjunto de coeficientes. La *teoría de Hartree-Fock* utiliza el Principio Variacional para resolver este problema. Este principio establece que para el estado fundamental de una función normalizada antisimétrica de las coordenadas electrónicas (la cual denotaremos como Ξ) el valor esperado de la energía será siempre mayor que el correspondiente a la función de onda exacta:

$$E(\Xi) > E(\psi), \quad \Xi \neq \psi \qquad \text{Ecuación 11}$$

En otras palabras, la energía de la función de onda exacta sirve como punto más bajo de las energías calculadas para cualquier otra función antisimétrica normalizada. Así, el problema se reduce a encontrar el conjunto de coeficientes que minimicen la energía de la función de onda resultante. Esto no se puede resolver analíticamente, por lo que resulta necesario recurrir al uso de un método iterativo conocido como *Método del Campo Autoconsistente* (*Self Consistent Field*, SCF). Cuando se alcanza la convergencia, la energía es un mínimo y los orbitales generan un campo que produce los mismos orbitales, de acuerdo con el nombre del método. La solución genera un conjunto de orbitales ocupados y desocupados, siendo el número de orbitales igual al número de las funciones base utilizadas.

Los métodos basados en la *teoría del Funcional de Densidad* se basan en la estrategia de modelar la correlación electrónica mediante unos funcionales generales de la densidad electrónica. Un funcional es una función, cuya definición es en sí una función; es decir, un funcional es una función de una función. Los métodos del funcional de densidad son una clase de métodos de estructura electrónica similares en muchos aspectos, a los métodos *ab initio*, en los que se requiere una cantidad de recursos computacionales superior a la teoría Hartree-Fock que es, desde el punto de vista computacional, el método menos costoso de los métodos *ab initio*. Los cálculos DFT son atractivos porque incluyen los efectos de la correlación electrónica, esto es, el hecho de que los electrones en un sistema molecular interaccionan desde el punto de vista electrostático; mientras que en los cálculos Hartree-Fock se promedia este efecto (cada electrón se ve afectado y reacciona con una densidad electrónica media), mientras que los métodos que incluyen la correlación electrónica tienen en cuenta las interacciones instantáneas de pares de electrones con espín opuesto. Esta aproximación provoca que los resultados obtenidos con la teoría Hartree - Fock sean menos exactos para algunos tipos de sistemas. La teoría del funcional de densidad utiliza una expresión más general de la energía que la teoría de Hartree - Fock. En ella se tienen en cuenta los funcionales de correlación e intercambio, que puede incluir términos que expliquen la energía de intercambio y la correlación electrónica que se omiten en la otra teoría:

$$E_{DFT} = V + \langle hP \rangle + {}^{1}/_{2} \langle PJ(P) \rangle + E_x[P] + E_c[P] \qquad \text{Ecuación 12}$$

donde $E_x[P]$ es el funcional de intercambio y $E_c[P]$, el funcional de correlación. Los funcionales de intercambio describen las interacciones entre electrones con el mismo espín, mientras que los de correlación describen las interacciones entre electrones de espín diferente. La teoría Hartree-Fock es, en realidad, un caso especial de la teoría del Funcional de Densidad, en el que $E_x[P]$ viene dado por la integral

de intercambio -½<PK(P)> y $E_c[P] = 0$. Los funcionales que se usan normalmente en la teoría del funcional de densidad son integrales de alguna función de la densidad y, en ocasiones, del gradiente de densidad:

$$E_x[P] = \int f\left(\boldsymbol{\rho_\alpha}(r), \boldsymbol{\rho_\beta}(r), \boldsymbol{\nabla\rho_\alpha}(r), \boldsymbol{\nabla\rho_\beta}(r)\right) dr \qquad \text{Ecuación 13}$$

Los funcionales locales dependen exclusivamente de la densidad electrónica ρ, mientras que los funcionales corregidos para el gradiente dependen tanto de ρ como de su gradiente $\nabla\rho$. Los funcionales híbridos formulados por Becke se definen de la siguiente manera:

$$E^{xc}_{híbrido} = c_{HF}\, E^{x}_{HF} + c_{DFT}\, E^{x}_{DFT} \qquad \text{Ecuación 14}$$

donde c_{HF} y c_{DFT} son constantes, E^{x}_{HF} es el término de intercambio tal y como se define en la teoría de HF y E^{x}_{DFT} representa el funcional de correlación e intercambio característico del método DFT.

Modelos de Solvatación

Mientras que las predicciones realizadas para fase gas son apropiadas para muchos propósitos, resultan inadecuadas para describir las características y propiedades de muchas moléculas y estados de transición en disolución. Por ejemplo, los efectos electrostáticos suelen ser mucho menos importantes para especies situadas en un disolvente con una elevada constante dieléctrica que para aquellas que se encuentran en fase gas. Los métodos que normalmente se emplean para modelar sistemas en disolución se conocen como *Métodos SCRF* (*Self-Consistent Reaction Field*). Todos ellos modelan el disolvente como un continuo de constante dieléctrica *ε* y consideran que el soluto está situado en el interior de una cavidad dentro del disolvente. Los métodos SCRF se diferencian entre sí en la manera de definir la cavidad y el medio de reacción (Figura 1).

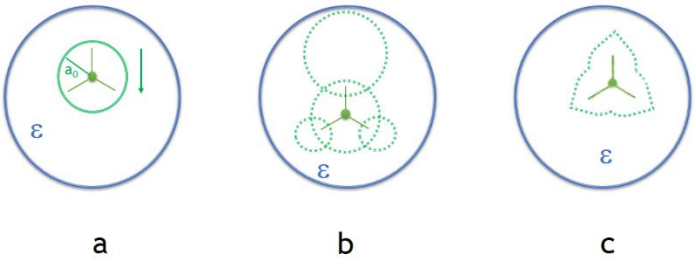


Figura 1. Representación esquemática de los diferentes modelos de solvatación empleados en el estudio de sistemas moleculares. a) Modelo de Onsager (dipolo y esfera); b) Modelo de Continuo Polarizado de Tomasi (PCM); c) Modelo PCM de isodensidad (IPCM).

El modelo SCFR más sencillo es el *modelo del campo de reacción de Onsager*. En este método, el soluto ocupa una cavidad esférica fija de radio a_0 dentro del campo de disolvente. Un dipolo en la molécula inducirá un dipolo en el medio, y el campo eléctrico aplicado por el dipolo del disolvente interaccionara

con el dipolo de la molécula, conduciendo a una estabilización neta. Hay que tener en cuenta que los sistemas que tienen un momento dipolar igual a cero no exhibirán efectos del disolvente para el modelo SCRF de Onsager y, por lo tanto, los cálculos llevados a cabo con el mismo darán los mismos resultados obtenidos en fase gas. Esta es una limitación intrínseca al enfoque del modelo de Onsager. El *modelo de continuo polarizado de Tomasi* (PCM) define la cavidad como la unión de una serie de esferas entrelazadas que engloban átomos o grupos de átomos. El efecto de la polarización del continuo disolvente se representa numéricamente y se calcula mediante integración numérica, en vez de mediante aproximación a la forma analítica usada en el modelo de Onsager. Por último, el *modelo PCM de isodensidad* (IPCM) define la cavidad como una superficie de la molécula con la misma densidad. Esta isodensidad se determina por un proceso interactivo en el que se realiza un ciclo SCF, que converge usando la superficie de isodensidad actual, la función de onda resultante se utiliza para calcular una superficie de isodensidad actualizada y el ciclo se repite hasta que la forma de la cavidad ya no cambia al terminar el ciclo SCF. Una superficie de isodensidad es una forma muy natural e intuitiva para la cavidad al corresponder a la forma reactiva de la molécula de la forma más precisa posible (en lugar de ser una forma predefinida más simple como una esfera o un conjunto de esferas entrelazadas).

Todos los cálculos se realizaron utilizando la Teoría del Funcional de Densidad (DFT) con la aproximación de meta gradiente generalizado (meta - GGA), el funcional de intercambio - correlación TPSSh y el paquete de programas Gaussian 09 (Revisión A.02). Para ello se emplearon los recursos computacionales del Centro de Supercomputación de Galicia (CESGA).

Complejos de 1,7-H_3Medo2ampa

Las geometrías optimizadas en disolución se corresponden con las siguientes conformaciones:

- F1: Δ(λλλλ)
- F2: Δ(δδδδ)
- F3: Δ(λλλδ)
- F4: Δ(λλδδ)
- F5: Δ(λδλδ)
- F6: Δ(δλλδ)
- F7: Δ(λδδδ)
- F8: Δ(δλδδ)
- F9: Δ(δδλδ)
- F10: Δ(ddδλ)
- F11: Δ(λλδλ)
- F12: Δ(λδδλ)
- F13: Δ(δλδλ)
- F14: Δ(λδλλ)
- F15: Δ(ddλλ)
- F16: Δ(δλλλ)

[La(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.111995	-1.655492	1.621014
2	6	0	1.271046	-2.596548	1.562019
3	6	0	2.595980	-1.922658	1.219031
4	7	0	2.635983	-1.290750	-0.126515
5	6	0	3.799783	-0.362715	-0.206253
6	6	0	3.608059	0.915532	0.607198
7	7	0	2.464169	1.738188	0.134676
8	6	0	2.019765	2.661412	1.211308
9	6	0	1.180534	1.974920	2.285835
10	7	0	-0.105184	1.387734	1.807171
11	6	0	-0.613598	0.440050	2.838635
12	6	0	0.171842	-0.869057	2.885169
13	6	0	2.761430	-2.334306	-1.177525
14	6	0	1.426056	-2.989670	-1.587433
15	8	0	1.452431	-4.151844	-2.015767
16	8	0	0.380526	-2.232231	-1.499367
17	6	0	-1.100037	2.471154	1.594953

18	6	0	-0.922735	3.238604	0.270660
19	8	0	-1.343970	4.399506	0.198516
20	8	0	-0.378640	2.559169	-0.688718
21	1	0	3.479013	-3.111184	-0.880194
22	1	0	3.153438	-1.852603	-2.080829
23	1	0	-2.093603	2.009419	1.552483
24	1	0	-1.100220	3.178756	2.435429
25	1	0	1.041837	-3.360722	0.817413
26	1	0	1.390896	-3.113549	2.526642
27	1	0	3.391564	-2.680706	1.296084
28	1	0	2.826075	-1.158177	1.963461
29	1	0	4.720060	-0.863732	0.132023
30	1	0	3.940695	-0.109387	-1.260798
31	1	0	4.539437	1.501280	0.560649
32	1	0	3.450357	0.675090	1.660787
33	1	0	2.891736	3.120546	1.704241
34	1	0	1.456775	3.469963	0.743525
35	1	0	1.766039	1.175597	2.744525
36	1	0	0.972537	2.705911	3.082729
37	1	0	-1.663887	0.238194	2.615383
38	1	0	-0.579454	0.900938	3.838075
39	1	0	1.221575	-0.665526	3.105488
40	1	0	-0.207750	-1.473519	3.722849
41	6	0	-1.134177	-2.464993	1.587206
42	1	0	-0.973615	-3.271487	0.864060
43	1	0	-1.324973	-2.930812	2.564386
44	6	0	-2.356711	-1.719521	1.106405
45	6	0	-3.631915	-1.955348	1.631786
46	6	0	-3.236104	-0.387163	-0.584342
47	6	0	-4.734835	-1.355234	1.019630
48	1	0	-3.753776	-2.599885	2.496114
49	6	0	-4.538759	-0.572279	-0.119156
50	1	0	-5.733141	-1.514676	1.415358
51	1	0	-5.360533	-0.113327	-0.656321
52	7	0	-2.167689	-0.921041	0.041108
53	6	0	-2.948013	0.359410	-1.878209
54	8	0	-3.877624	0.934861	-2.460153
55	8	0	-1.715540	0.281413	-2.268079

56	6	0	2.900135	2.550774	-1.026776
57	1	0	2.059893	3.156476	-1.369321
58	1	0	3.736234	3.212576	-0.753231
59	1	0	3.219743	1.897972	-1.842105
60	8	0	0.415646	1.605316	-3.025073
61	1	0	0.183424	2.371908	-2.449268
62	1	0	-0.478739	1.220944	-3.199946
63	57	0	0.257620	0.096659	-0.650238

E(RTPSSh) = -1612.50378331

Zero-point correction= 0.518364 (Hartree/Particle)

Thermal correction to Energy= 0.549808

Thermal correction to Enthalpy= 0.550752

Thermal correction to Gibbs Free Energy= 0.458803

Sum of electronic and zero-point Energies= -1611.985419

Sum of electronic and thermal Energies= -1611.953975

Sum of electronic and thermal Enthalpies= -1611.953031

Sum of electronic and thermal Free Energies= -1612.044981

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.243047	-0.886591	2.094043
2	6	0	0.875142	-1.793638	2.480420
3	6	0	1.267463	-2.773318	1.371918
4	7	0	1.877239	-2.119833	0.183164
5	6	0	3.281349	-1.725192	0.473041
6	6	0	3.782523	-0.620498	-0.453545
7	7	0	3.010025	0.642881	-0.339572
8	6	0	3.320181	1.307388	0.949645
9	6	0	2.320993	2.396036	1.317364
10	7	0	0.943974	1.869964	1.519300
11	6	0	0.814853	1.288200	2.877912
12	6	0	-0.333644	0.290800	3.009290
13	6	0	1.867203	-3.081625	-0.946836
14	6	0	0.512156	-3.175597	-1.671074

15	8	0	0.203374	-4.246703	-2.208533
16	8	0	-0.176482	-2.077782	-1.708632
17	6	0	-0.010363	2.984329	1.324121
18	6	0	-0.075143	3.431606	-0.151783
19	8	0	-0.514617	4.557653	-0.411819
20	8	0	0.323548	2.545026	-1.011913
21	1	0	2.181405	-4.080372	-0.613771
22	1	0	2.595762	-2.742183	-1.691224
23	1	0	-1.012899	2.642750	1.609103
24	1	0	0.236502	3.847235	1.959480
25	6	0	-1.515348	-1.644666	2.216062
26	1	0	-1.364743	-2.634643	1.773167
27	1	0	-1.766661	-1.803533	3.274941
28	6	0	-2.673132	-0.999071	1.491874
29	6	0	-3.984612	-1.107451	1.967717
30	6	0	-3.400630	0.058276	-0.444073
31	6	0	-5.028889	-0.605346	1.189732
32	1	0	-4.177860	-1.584104	2.923126
33	6	0	-4.734270	-0.021420	-0.042681
34	1	0	-6.054895	-0.678317	1.536804
35	1	0	-5.502526	0.367185	-0.700842
36	1	0	2.278517	3.145131	0.524554
37	1	0	2.667984	2.909706	2.227115
38	1	0	3.335070	0.549264	1.735481
39	1	0	4.330698	1.746508	0.916630
40	1	0	0.664347	2.080344	3.627608
41	1	0	1.762292	0.804927	3.129702
42	1	0	-0.381085	-0.049964	4.055215
43	1	0	-1.285681	0.785001	2.789643
44	1	0	0.603534	-2.366782	3.379847
45	1	0	1.734244	-1.177825	2.752513
46	1	0	0.389321	-3.326054	1.023677
47	1	0	1.960678	-3.517309	1.794252
48	1	0	3.342963	-1.403793	1.514683
49	1	0	3.948382	-2.595587	0.380519
50	1	0	4.850134	-0.441522	-0.244539
51	1	0	3.713834	-0.946999	-1.496231
52	7	0	-2.388798	-0.406135	0.318533

53	6	0	-3.026762	0.628788	-1.802521
54	8	0	-3.926632	1.058204	-2.537911
55	8	0	-1.762998	0.588713	-2.071310
56	6	0	3.403485	1.527515	-1.460615
57	1	0	2.830663	2.454929	-1.417599
58	1	0	4.479338	1.760932	-1.423590
59	1	0	3.178317	1.028553	-2.406022
60	8	0	0.596789	1.003983	-3.149432
61	1	0	0.629710	1.896087	-2.729886
62	1	0	-0.375479	0.874128	-3.256721
63	57	0	0.173565	0.054927	-0.539567

E(RTPSSh) = -1612.50737647

Zero-point correction= 0.518103 (Hartree/Particle)

Thermal correction to Energy= 0.549775

Thermal correction to Enthalpy= 0.550720

Thermal correction to Gibbs Free Energy= 0.457951

Sum of electronic and zero-point Energies= -1611.989273

Sum of electronic and thermal Energies= -1611.957601

Sum of electronic and thermal Enthalpies= -1611.956657

Sum of electronic and thermal Free Energies= -1612.049425

[Nd(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.093164	-1.631480	1.649640
2	6	0	1.240292	-2.585668	1.589892
3	6	0	2.565221	-1.919979	1.233534
4	7	0	2.590395	-1.286881	-0.113762
5	6	0	3.761666	-0.368925	-0.202851
6	6	0	3.570414	0.912043	0.604260
7	7	0	2.424958	1.727627	0.122079
8	6	0	1.986295	2.667151	1.187571

9	6	0	1.154814	1.997206	2.276080
10	7	0	-0.123116	1.388104	1.804471
11	6	0	-0.626614	0.462969	2.857319
12	6	0	0.162172	-0.842817	2.912018
13	6	0	2.698115	-2.336480	-1.161346
14	6	0	1.347210	-2.964279	-1.556286
15	8	0	1.336688	-4.129822	-1.972996
16	8	0	0.322151	-2.177054	-1.465669
17	6	0	-1.122757	2.459983	1.554708
18	6	0	-0.927703	3.180291	0.207036
19	8	0	-1.311258	4.350343	0.093516
20	8	0	-0.407107	2.450673	-0.729989
21	1	0	3.403144	-3.123992	-0.863455
22	1	0	3.093342	-1.865050	-2.068517
23	1	0	-2.114313	1.993511	1.518979
24	1	0	-1.130060	3.193911	2.371812
25	1	0	0.999554	-3.351803	0.850711
26	1	0	1.362130	-3.098281	2.556257
27	1	0	3.358680	-2.680679	1.299290
28	1	0	2.807216	-1.156915	1.975508
29	1	0	4.678191	-0.874005	0.138257
30	1	0	3.902568	-0.122082	-1.258751
31	1	0	4.499927	1.500291	0.557356
32	1	0	3.409267	0.676332	1.658310
33	1	0	2.860800	3.135484	1.666728
34	1	0	1.419248	3.468652	0.711725
35	1	0	1.746106	1.213621	2.754206
36	1	0	0.936276	2.743518	3.055448
37	1	0	-1.678641	0.257521	2.646355
38	1	0	-0.583478	0.941348	3.847725
39	1	0	1.212939	-0.634994	3.123372
40	1	0	-0.210340	-1.445257	3.754031
41	6	0	-1.167757	-2.417243	1.619767
42	1	0	-1.018948	-3.240821	0.913369
43	1	0	-1.377811	-2.861099	2.602889
44	6	0	-2.367005	-1.653179	1.110628
45	6	0	-3.661106	-1.881353	1.591490
46	6	0	-3.181889	-0.318246	-0.610990

47	6	0	-4.738346	-1.271261	0.944778
48	1	0	-3.817005	-2.529619	2.447444
49	6	0	-4.499859	-0.492454	-0.189292
50	1	0	-5.750340	-1.424193	1.306690
51	1	0	-5.300930	-0.033883	-0.757222
52	7	0	-2.137599	-0.850750	0.056263
53	6	0	-2.837692	0.390311	-1.911257
54	8	0	-3.729423	0.981698	-2.533835
55	8	0	-1.599549	0.251607	-2.264412
56	6	0	2.869188	2.530805	-1.042523
57	1	0	2.040880	3.156327	-1.378469
58	1	0	3.717881	3.177383	-0.771535
59	1	0	3.170848	1.873485	-1.860131
60	8	0	0.647599	1.366714	-2.923655
61	1	0	0.395088	2.194761	-2.453508
62	1	0	-0.242369	1.023932	-3.186325
63	60	0	0.247580	0.073662	-0.591671

E(RTPSSh) = -1614.40754698

Zero-point correction= 0.518850 (Hartree/Particle)

Thermal correction to Energy= 0.550246

Thermal correction to Enthalpy= 0.551190

Thermal correction to Gibbs Free Energy= 0.459415

Sum of electronic and zero-point Energies= -1613.888697

Sum of electronic and thermal Energies= -1613.857301

Sum of electronic and thermal Enthalpies= -1613.856357

Sum of electronic and thermal Free Energies= -1613.948132

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.245713	-0.846829	2.115660
2	6	0	0.867659	-1.752571	2.515148
3	6	0	1.247579	-2.745230	1.416465
4	7	0	1.840713	-2.100095	0.214929
5	6	0	3.252951	-1.718353	0.479713

6	6	0	3.742025	-0.627617	-0.467033
7	7	0	2.965414	0.634543	-0.359798
8	6	0	3.288532	1.309694	0.922049
9	6	0	2.295922	2.406005	1.278637
10	7	0	0.921573	1.879567	1.498704
11	6	0	0.802219	1.334604	2.872441
12	6	0	-0.339296	0.334684	3.024127
13	6	0	1.806745	-3.071631	-0.906583
14	6	0	0.439502	-3.145852	-1.604222
15	8	0	0.096913	-4.208826	-2.136074
16	8	0	-0.226944	-2.033738	-1.625296
17	6	0	-0.035667	2.986405	1.272668
18	6	0	-0.102282	3.378383	-0.217951
19	8	0	-0.542606	4.492609	-0.522030
20	8	0	0.302467	2.460914	-1.043298
21	1	0	2.112566	-4.071242	-0.569184
22	1	0	2.527840	-2.747691	-1.664888
23	1	0	-1.036487	2.661100	1.580719
24	1	0	0.219649	3.871155	1.873775
25	6	0	-1.521195	-1.597939	2.240494
26	1	0	-1.374176	-2.596759	1.817076
27	1	0	-1.784543	-1.735124	3.299295
28	6	0	-2.659972	-0.951960	1.490585
29	6	0	-3.978066	-1.025244	1.953432
30	6	0	-3.344285	0.075233	-0.475221
31	6	0	-5.003820	-0.519041	1.153955
32	1	0	-4.189860	-1.476441	2.917256
33	6	0	-4.683691	0.029275	-0.088325
34	1	0	-6.034443	-0.561879	1.492257
35	1	0	-5.436537	0.417213	-0.764433
36	1	0	2.248259	3.141114	0.473266
37	1	0	2.647783	2.935145	2.177240
38	1	0	3.303205	0.561244	1.717075
39	1	0	4.301559	1.741108	0.876607
40	1	0	0.650500	2.144404	3.602462
41	1	0	1.753025	0.861805	3.131894

42	1	0	-0.378308	0.000558	4.072379
43	1	0	-1.294987	0.822780	2.806915
44	1	0	0.595747	-2.311419	3.423340
45	1	0	1.731054	-1.137136	2.774981
46	1	0	0.366172	-3.302537	1.084587
47	1	0	1.947779	-3.483842	1.836012
48	1	0	3.334471	-1.388275	1.517071
49	1	0	3.909650	-2.595874	0.383183
50	1	0	4.811114	-0.441434	-0.273713
51	1	0	3.661112	-0.967726	-1.504390
52	7	0	-2.348634	-0.388288	0.309089
53	6	0	-2.938979	0.602665	-1.840254
54	8	0	-3.820221	1.004219	-2.613390
55	8	0	-1.668886	0.559107	-2.072026
56	6	0	3.369796	1.510467	-1.485296
57	1	0	2.793701	2.436403	-1.458183
58	1	0	4.443939	1.747881	-1.433665
59	1	0	3.160684	1.000237	-2.427460
60	8	0	0.755376	0.748556	-3.019169
61	1	0	0.761023	1.688613	-2.722361
62	1	0	-0.199525	0.615585	-3.227211
63	60	0	0.171862	0.047736	-0.503678

E(RTPSSh) = -1614.41100358

Zero-point correction= 0.518767 (Hartree/Particle)

Thermal correction to Energy= 0.550150

Thermal correction to Enthalpy= 0.551094

Thermal correction to Gibbs Free Energy= 0.459594

Sum of electronic and zero-point Energies= -1613.892236

Sum of electronic and thermal Energies= -1613.860854

Sum of electronic and thermal Enthalpies= -1613.859909

Sum of electronic and thermal Free Energies= -1613.951410

[Eu(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.143341	-1.526734	1.731652
2	6	0	1.322239	-2.443775	1.705551
3	6	0	2.627138	-1.740621	1.343242
4	7	0	2.639113	-1.137826	-0.017681
5	6	0	3.760544	-0.161742	-0.116101
6	6	0	3.468452	1.140548	0.622173
7	7	0	2.277530	1.846634	0.078728
8	6	0	1.766283	2.826099	1.074562
9	6	0	0.971893	2.178949	2.202961
10	7	0	-0.250805	1.444389	1.767321
11	6	0	-0.684533	0.550624	2.875298
12	6	0	0.184642	-0.698569	2.968773
13	6	0	2.802065	-2.202306	-1.041422
14	6	0	1.479901	-2.890844	-1.428896
15	8	0	1.516684	-4.058984	-1.836224
16	8	0	0.422789	-2.146820	-1.341187
17	6	0	-1.328752	2.411078	1.439894
18	6	0	-1.166379	3.042022	0.044760
19	8	0	-1.634548	4.170543	-0.157269
20	8	0	-0.579633	2.289959	-0.829599
21	1	0	3.536304	-2.953725	-0.721969
22	1	0	3.184042	-1.734082	-1.955626
23	1	0	-2.279145	1.865268	1.430338
24	1	0	-1.404987	3.198639	2.201996
25	1	0	1.114205	-3.235323	0.983506
26	1	0	1.452468	-2.926951	2.685756
27	1	0	3.445429	-2.472010	1.431365
28	1	0	2.838886	-0.951994	2.067884
29	1	0	4.692712	-0.596170	0.275487
30	1	0	3.921943	0.043432	-1.177759

31	1	0	4.354988	1.790655	0.563147
32	1	0	3.298653	0.944929	1.683388
33	1	0	2.604570	3.382935	1.522018
34	1	0	1.152244	3.552219	0.539871
35	1	0	1.610778	1.474286	2.739340
36	1	0	0.691369	2.960688	2.925232
37	1	0	-1.725499	0.271890	2.695086
38	1	0	-0.654551	1.080133	3.839542
39	1	0	1.223327	-0.417213	3.153113
40	1	0	-0.135722	-1.296243	3.835233
41	6	0	-1.095977	-2.347501	1.726714
42	1	0	-0.913201	-3.207021	1.072954
43	1	0	-1.312510	-2.738985	2.730132
44	6	0	-2.304317	-1.646529	1.150363
45	6	0	-3.606784	-1.906749	1.591263
46	6	0	-3.102796	-0.418492	-0.658694
47	6	0	-4.679670	-1.363680	0.880806
48	1	0	-3.771852	-2.529033	2.464669
49	6	0	-4.427945	-0.625105	-0.277847
50	1	0	-5.698372	-1.541534	1.211145
51	1	0	-5.224348	-0.227383	-0.895988
52	7	0	-2.067060	-0.875843	0.074953
53	6	0	-2.727139	0.217500	-1.988062
54	8	0	-3.604225	0.754171	-2.676570
55	8	0	-1.476893	0.066810	-2.287943
56	63	0	0.244808	0.068145	-0.528184
57	6	0	2.674690	2.605229	-1.131347
58	1	0	1.789655	3.096290	-1.542549
59	1	0	3.426639	3.370630	-0.886748
60	1	0	3.101170	1.930223	-1.876842
61	8	0	0.906746	0.669560	-2.968714
62	1	0	1.116861	1.608589	-3.115006
63	1	0	-0.062478	0.590639	-3.171853

E(RTPSSh) = -1616.22395134

Zero-point correction= 0.518453 (Hartree/Particle)

Thermal correction to Energy= 0.550023

Thermal correction to Enthalpy= 0.550967

Thermal correction to Gibbs Free Energy= 0.458790

Sum of electronic and zero-point Energies= -1615.705499

Sum of electronic and thermal Energies= -1615.673928

Sum of electronic and thermal Enthalpies= -1615.672984

Sum of electronic and thermal Free Energies= -1615.765161

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.243321	-0.910720	2.070797
2	6	0	0.865490	-1.829448	2.452578
3	6	0	1.240055	-2.795651	1.331589
4	7	0	1.805657	-2.113656	0.137225
5	6	0	3.234464	-1.777336	0.367651
6	6	0	3.711952	-0.652494	-0.543273
7	7	0	2.943015	0.608827	-0.373822
8	6	0	3.275255	1.217077	0.939303
9	6	0	2.306457	2.318386	1.336983
10	7	0	0.922981	1.804928	1.540516
11	6	0	0.800228	1.235087	2.904572
12	6	0	-0.341248	0.234284	3.024011
13	6	0	1.697546	-3.032201	-1.022113
14	6	0	0.272798	-3.082841	-1.595569
15	8	0	-0.081939	-4.085905	-2.225963
16	8	0	-0.437118	-2.015222	-1.397952
17	6	0	-0.013271	2.935365	1.342031
18	6	0	-0.065283	3.351853	-0.142274
19	8	0	-0.487965	4.475721	-0.434609
20	8	0	0.337088	2.440214	-0.975448
21	1	0	2.034377	-4.044425	-0.759120
22	1	0	2.354121	-2.665701	-1.819018
23	1	0	-1.020104	2.624681	1.645097

24	1	0	0.262156	3.802092	1.959689
25	6	0	-1.522826	-1.657516	2.156250
26	1	0	-1.386755	-2.631462	1.675436
27	1	0	-1.787966	-1.850419	3.205899
28	6	0	-2.650138	-0.956478	1.440779
29	6	0	-3.976730	-1.062049	1.872220
30	6	0	-3.298712	0.184135	-0.471738
31	6	0	-4.987446	-0.504062	1.088244
32	1	0	-4.206342	-1.578744	2.798327
33	6	0	-4.645006	0.116768	-0.113740
34	1	0	-6.024298	-0.568512	1.403340
35	1	0	-5.386390	0.538342	-0.782436
36	1	0	2.271958	3.084734	0.560879
37	1	0	2.665976	2.806075	2.255236
38	1	0	3.264747	0.433608	1.699799
39	1	0	4.299169	1.623655	0.918312
40	1	0	0.646722	2.031339	3.648207
41	1	0	1.749851	0.756580	3.157777
42	1	0	-0.381655	-0.139245	4.058676
43	1	0	-1.295971	0.731495	2.824077
44	1	0	0.590050	-2.405803	3.348682
45	1	0	1.731806	-1.223056	2.724984
46	1	0	0.360428	-3.356789	1.003863
47	1	0	1.956147	-3.533666	1.723609
48	1	0	3.360030	-1.503100	1.417259
49	1	0	3.867927	-2.661716	0.203403
50	1	0	4.784754	-0.477174	-0.361862
51	1	0	3.610059	-0.951266	-1.591361
52	7	0	-2.317227	-0.315064	0.306972
53	6	0	-2.863245	0.745021	-1.811859
54	8	0	-3.717158	1.214867	-2.577057
55	8	0	-1.595798	0.638940	-2.038256
56	63	0	0.184126	0.065239	-0.472324
57	6	0	3.367605	1.534396	-1.452272
58	1	0	2.792677	2.459523	-1.394380
59	1	0	4.440713	1.766326	-1.368867

60	1	0	3.178675	1.065756	-2.419712
61	8	0	0.821982	0.689805	-2.921236
62	1	0	0.860754	1.635512	-2.647779
63	1	0	-0.131689	0.599950	-3.159507

E(RTPSSh) = -1616.22649910

Zero-point correction= 0.518608 (Hartree/Particle)

Thermal correction to Energy= 0.550182

Thermal correction to Enthalpy= 0.551126

Thermal correction to Gibbs Free Energy= 0.458744

Sum of electronic and zero-point Energies= -1615.707891

Sum of electronic and thermal Energies= -1615.676317

Sum of electronic and thermal Enthalpies= -1615.675373

Sum of electronic and thermal Free Energies= -1615.767755

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.169400	-1.108040	2.036870
2	7	0	2.038383	-1.939961	0.015038
3	6	0	3.427232	-1.456314	0.272975
4	6	0	3.504151	-0.081482	0.936372
5	7	0	2.769153	0.965152	0.184877
6	6	0	2.614344	2.178379	1.029788
7	6	0	1.517977	2.034593	2.081318
8	7	0	0.154871	1.795782	1.529141
9	6	0	-0.742392	1.300146	2.606995
10	6	0	-0.351820	-0.088223	3.119431
11	6	0	2.029458	-2.804135	-1.195685
12	6	0	0.605761	-3.020355	-1.740503
13	8	0	0.385728	-4.009770	-2.449114
14	8	0	-0.247799	-2.093090	-1.433717
15	6	0	-0.392425	3.055818	0.963240
16	6	0	0.132730	3.372003	-0.449376

17	8	0	0.101378	4.541094	-0.849757
18	8	0	0.534229	2.341632	-1.126494
19	1	0	2.506336	-3.774822	-1.003242
20	1	0	2.602777	-2.301202	-1.982097
21	1	0	-1.479873	2.945027	0.878674
22	1	0	-0.200453	3.907767	1.629723
23	1	0	3.977847	-2.178357	0.892508
24	1	0	3.941666	-1.415228	-0.690056
25	1	0	4.567122	0.193154	1.036042
26	1	0	3.096237	-0.123816	1.947212
27	1	0	3.558476	2.404485	1.550623
28	1	0	2.406529	3.019906	0.368171
29	1	0	1.763442	1.200900	2.740748
30	1	0	1.509528	2.939494	2.708310
31	1	0	-1.756195	1.282320	2.200607
32	1	0	-0.746448	1.991058	3.464927
33	1	0	0.574373	-0.031605	3.695216
34	1	0	-1.124827	-0.419774	3.824684
35	6	0	-1.394856	-1.938875	1.936609
36	1	0	-1.173610	-2.795356	1.291049
37	1	0	-1.679374	-2.331321	2.923202
38	6	0	-2.544414	-1.194869	1.304110
39	6	0	-3.864088	-1.324737	1.745781
40	6	0	-4.882198	-0.698355	1.022358
41	6	0	-3.215490	0.086370	-0.514756
42	6	0	-4.556546	0.003370	-0.138574
43	1	0	-5.306210	0.477263	-0.761455
44	1	0	-4.085449	-1.907415	2.633705
45	1	0	-5.913746	-0.774387	1.351844
46	6	0	0.994385	-1.991576	2.346831
47	6	0	1.508325	-2.768192	1.138053
48	1	0	1.788144	-1.365888	2.756646
49	1	0	0.728323	-2.715933	3.131404
50	1	0	2.287791	-3.463389	1.485185
51	1	0	0.700494	-3.381421	0.729735
52	6	0	-2.789788	0.731870	-1.821976

53	8	0	-3.650651	1.258915	-2.540390
54	8	0	-1.525990	0.630207	-2.073252
55	7	0	-2.228267	-0.468700	0.215928
56	63	0	0.222525	0.032258	-0.493451
57	6	0	3.530473	1.334716	-1.030628
58	1	0	2.992017	2.126885	-1.552451
59	1	0	4.539828	1.690389	-0.771902
60	1	0	3.619630	0.474437	-1.696887
61	8	0	0.966830	0.498956	-2.938546
62	1	0	1.001442	1.458609	-2.707864
63	1	0	0.037253	0.401842	-3.243855

E(RTPSSh) = -1616.22207293

Zero-point correction= 0.518600 (Hartree/Particle)

Thermal correction to Energy= 0.550326

Thermal correction to Enthalpy= 0.551270

Thermal correction to Gibbs Free Energy= 0.458121

Sum of electronic and zero-point Energies= -1615.703473

Sum of electronic and thermal Energies= -1615.671747

Sum of electronic and thermal Enthalpies= -1615.670803

Sum of electronic and thermal Free Energies= -1615.763952

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.495109	-1.306632	2.030212
2	7	0	1.830450	-1.996456	0.211211
3	7	0	2.819124	0.862078	0.075945
4	6	0	2.780947	1.690077	1.320012
5	6	0	1.658788	1.357869	2.303582
6	7	0	0.291800	1.526599	1.740398
7	6	0	-0.742792	1.103976	2.723366
8	6	0	-0.607986	-0.347871	3.170089
9	6	0	2.146858	-2.681402	-1.066786

10	6	0	0.904737	-2.836582	-1.963423
11	8	0	0.883019	-3.746624	-2.799478
12	8	0	-0.014912	-1.938815	-1.785308
13	6	0	0.045566	2.953633	1.403706
14	6	0	0.532196	3.348064	0.002333
15	8	0	0.907895	4.507307	-0.210718
16	8	0	0.457856	2.399707	-0.878416
17	1	0	2.605793	-3.663349	-0.886610
18	1	0	2.868698	-2.076631	-1.624728
19	1	0	-1.038175	3.115374	1.412310
20	1	0	0.483526	3.619635	2.159002
21	1	0	3.736491	1.604106	1.858293
22	1	0	2.690959	2.736138	1.015551
23	1	0	1.760320	0.325220	2.640518
24	1	0	1.782489	2.000436	3.190239
25	1	0	-1.713831	1.262715	2.245869
26	1	0	-0.706984	1.741956	3.620755
27	1	0	0.268121	-0.461244	3.812516
28	1	0	-1.476624	-0.593742	3.794956
29	6	0	-1.804961	-1.960345	1.792157
30	1	0	-1.636101	-2.817872	1.130713
31	1	0	-2.217888	-2.352348	2.732925
32	6	0	-2.810948	-1.066238	1.110400
33	6	0	-4.155105	-1.038736	1.493436
34	6	0	-5.061142	-0.294037	0.734832
35	6	0	-3.246211	0.298726	-0.718599
36	6	0	-4.603038	0.371887	-0.401464
37	1	0	-5.261989	0.935903	-1.050996
38	1	0	-4.480937	-1.596899	2.364873
39	1	0	-6.108190	-0.251707	1.018189
40	6	0	0.505356	-2.369922	2.325936
41	6	0	1.105299	-2.976132	1.064612
42	1	0	1.290414	-1.936510	2.948341
43	1	0	0.054191	-3.177355	2.921431
44	1	0	1.781210	-3.795624	1.355711
45	1	0	0.315141	-3.414072	0.447267

46	6	0	3.704252	-0.330563	0.208606
47	6	0	3.074171	-1.540964	0.885568
48	1	0	4.012830	-0.604339	-0.803900
49	1	0	4.622780	-0.065586	0.754645
50	1	0	3.817564	-2.353089	0.907594
51	1	0	2.838926	-1.305687	1.923936
52	7	0	-2.361346	-0.378777	0.041991
53	6	0	-2.698860	0.915192	-1.993905
54	8	0	-3.467991	1.535056	-2.740721
55	8	0	-1.440902	0.690977	-2.189696
56	63	0	0.170658	0.040856	-0.509933
57	6	0	3.430022	1.700991	-0.992924
58	1	0	2.844494	2.611665	-1.122100
59	1	0	4.465279	1.970823	-0.734708
60	1	0	3.433539	1.141992	-1.930724
61	8	0	1.096885	0.764707	-2.821754
62	1	0	1.117173	1.691447	-2.481991
63	1	0	0.187224	0.702744	-3.192855

E(RTPSSh) = -1616.21799374

Zero-point correction= 0.519045 (Hartree/Particle)

Thermal correction to Energy= 0.550562

Thermal correction to Enthalpy= 0.551506

Thermal correction to Gibbs Free Energy= 0.459284

Sum of electronic and zero-point Energies= -1615.698949

Sum of electronic and thermal Energies= -1615.667432

Sum of electronic and thermal Enthalpies= -1615.666488

Sum of electronic and thermal Free Energies= -1615.758710

F5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.258826	-0.982009	1.992869
2	7	0	2.285981	-1.641930	-0.254321

3	6	0	3.617641	-0.977669	-0.294450
4	6	0	3.742071	0.208669	0.652748
5	7	0	2.670278	1.214516	0.417891
6	6	0	-0.716024	1.292528	2.581571
7	6	0	0.050557	0.053907	3.057533
8	6	0	2.194142	-2.570750	-1.412597
9	6	0	0.741603	-2.984181	-1.704108
10	8	0	0.531193	-4.043108	-2.307218
11	8	0	-0.155339	-2.131381	-1.316400
12	6	0	-1.142975	2.790498	0.698291
13	6	0	-0.710526	3.160554	-0.737842
14	8	0	-1.273955	4.102458	-1.303271
15	8	0	0.225261	2.408673	-1.236001
16	1	0	2.817977	-3.462401	-1.264338
17	1	0	2.567925	-2.047273	-2.299785
18	1	0	-2.096974	2.254297	0.636449
19	1	0	-1.320026	3.707496	1.277299
20	1	0	4.417007	-1.701491	-0.073442
21	1	0	3.765839	-0.634822	-1.322904
22	1	0	4.734127	0.663049	0.512513
23	1	0	3.705054	-0.120460	1.691443
24	1	0	-1.752462	1.027975	2.363074
25	1	0	-0.736048	2.019710	3.407707
26	1	0	1.027529	0.347500	3.441362
27	1	0	-0.493289	-0.383052	3.906087
28	6	0	-0.842075	-1.979929	2.053396
29	1	0	-0.555966	-2.829653	1.424408
30	1	0	-0.966103	-2.352026	3.079957
31	6	0	-2.145910	-1.456797	1.507368
32	6	0	-3.387634	-1.827583	2.031155
33	6	0	-4.547281	-1.412906	1.371363
34	6	0	-3.156411	-0.343068	-0.265068
35	6	0	-4.431799	-0.675615	0.192148
36	1	0	-5.294183	-0.361045	-0.383789
37	1	0	-3.440114	-2.432620	2.930123
38	1	0	-5.523738	-1.679742	1.763516

39	6	0	1.550299	-1.698878	2.214429
40	6	0	2.072658	-2.449429	0.985598
41	1	0	2.276742	-0.964100	2.555089
42	1	0	1.446584	-2.432299	3.028456
43	1	0	3.012108	-2.946718	1.270452
44	1	0	1.367542	-3.244425	0.728217
45	6	0	2.398265	1.974313	1.662411
46	6	0	1.071604	2.729579	1.631495
47	7	0	-0.145509	1.903907	1.354069
48	1	0	1.126165	3.493217	0.853648
49	1	0	0.946494	3.254723	2.589723
50	1	0	2.425240	1.273043	2.497146
51	1	0	3.196348	2.710760	1.850818
52	7	0	-2.041412	-0.693961	0.404633
53	6	0	-2.931188	0.358898	-1.593961
54	8	0	-3.917041	0.700153	-2.263806
55	8	0	-1.687830	0.506994	-1.911133
56	63	0	0.246331	0.073979	-0.513919
57	6	0	3.136312	2.142056	-0.645261
58	1	0	2.359006	2.871001	-0.867681
59	1	0	4.058856	2.653901	-0.331724
60	1	0	3.340444	1.575382	-1.557644
61	8	0	0.874397	0.549688	-2.972553
62	1	0	0.661211	1.496781	-2.768904
63	1	0	0.057241	0.225972	-3.400600

E(RTPSSh) = -1616.21763610

Zero-point correction= 0.518186 (Hartree/Particle)

Thermal correction to Energy= 0.549908

Thermal correction to Enthalpy= 0.550852

Thermal correction to Gibbs Free Energy= 0.458506

Sum of electronic and zero-point Energies= -1615.699450

Sum of electronic and thermal Energies= -1615.667728

Sum of electronic and thermal Enthalpies= -1615.666784

Sum of electronic and thermal Free Energies= -1615.759130

F6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.204993	-0.745279	2.099987
2	6	0	0.929552	-1.604563	2.542923
3	6	0	1.332822	-2.637329	1.493627
4	7	0	1.882831	-2.065924	0.232158
5	6	0	3.321113	-1.689785	0.367999
6	6	0	3.532499	-0.194433	0.586966
7	7	0	2.856895	0.643652	-0.431764
8	7	0	0.978850	1.928793	1.457437
9	6	0	1.722883	-3.095282	-0.825265
10	6	0	0.264392	-3.220584	-1.297438
11	8	0	-0.446369	-2.143141	-1.177999
12	8	0	-0.112653	-4.291173	-1.789831
13	6	0	0.011343	3.010150	1.148933
14	6	0	-0.021305	3.341704	-0.353899
15	8	0	-0.314436	4.492438	-0.705786
16	8	0	0.233605	2.343779	-1.137140
17	1	0	2.091563	-4.076787	-0.496650
18	1	0	2.317676	-2.794245	-1.694510
19	1	0	-0.994275	2.676992	1.434141
20	1	0	0.235853	3.917003	1.728216
21	1	0	0.664768	-2.130410	3.472915
22	1	0	1.778845	-0.962004	2.777972
23	1	0	0.463669	-3.242357	1.220903
24	1	0	2.063876	-3.324460	1.945296
25	1	0	3.786208	-2.233143	1.201285
26	1	0	3.844577	-2.007659	-0.536733
27	1	0	4.615179	0.014225	0.602949
28	1	0	3.137145	0.085243	1.564900
29	6	0	-1.464987	-1.523629	2.225429
30	1	0	-1.308578	-2.505462	1.768557
31	1	0	-1.711780	-1.689708	3.284045

32	6	0	-2.617301	-0.869534	1.503797
33	6	0	-3.932732	-0.938068	1.974481
34	6	0	-4.958188	-0.412644	1.185739
35	6	0	-3.306401	0.169522	-0.454176
36	6	0	-4.643368	0.138032	-0.057424
37	1	0	-5.399118	0.532563	-0.726635
38	1	0	-4.143748	-1.397296	2.934643
39	1	0	-5.986702	-0.446657	1.531477
40	6	0	0.790058	1.454482	2.851983
41	6	0	-0.346239	0.449915	2.983466
42	1	0	-0.416849	0.133951	4.035776
43	1	0	-1.299561	0.922359	2.726382
44	1	0	1.726511	1.001180	3.186630
45	1	0	0.590913	2.293349	3.535947
46	6	0	2.369552	2.443659	1.266314
47	6	0	2.998711	2.079746	-0.080168
48	1	0	2.992313	2.061263	2.078551
49	1	0	2.384803	3.537866	1.363383
50	1	0	2.534594	2.646600	-0.887235
51	1	0	4.065824	2.356190	-0.035416
52	7	0	-2.312551	-0.297753	0.326820
53	6	0	-2.895082	0.653404	-1.832456
54	8	0	-3.757904	1.102911	-2.599539
55	8	0	-1.635480	0.507240	-2.081128
56	63	0	0.178130	0.042450	-0.500281
57	6	0	3.492752	0.446985	-1.755373
58	1	0	4.574497	0.646752	-1.705999
59	1	0	3.337942	-0.575433	-2.105082
60	1	0	3.030115	1.124554	-2.473739
61	8	0	0.704479	0.104390	-3.039423
62	1	0	-0.247051	0.351524	-3.167271
63	1	0	0.790969	-0.776824	-3.445454

E(RTPSSh) = -1616.21622484

Zero-point correction= 0.518463 (Hartree/Particle)

Thermal correction to Energy= 0.550129

Thermal correction to Enthalpy= 0.551073

Thermal correction to Gibbs Free Energy= 0.458583

Sum of electronic and zero-point Energies= -1615.697762

Sum of electronic and thermal Energies= -1615.666096

Sum of electronic and thermal Enthalpies= -1615.665152

Sum of electronic and thermal Free Energies= -1615.757642

F7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.078960	-1.157952	2.093508
2	7	0	2.394515	-1.507940	0.172247
3	7	0	2.462308	1.466100	0.221465
4	6	0	2.195714	1.775413	1.649230
5	6	0	0.868010	2.498443	1.901209
6	7	0	-0.373108	1.741665	1.531968
7	6	0	-0.972811	1.045490	2.699035
8	6	0	-0.149548	-0.147841	3.167365
9	6	0	2.775885	-2.191294	-1.089830
10	6	0	1.557739	-2.633089	-1.919109
11	8	0	1.690139	-3.570405	-2.714885
12	8	0	0.482387	-1.930331	-1.739952
13	6	0	-1.365550	2.704821	0.985903
14	6	0	-0.965577	3.195789	-0.416282
15	8	0	-1.455697	4.243322	-0.852048
16	8	0	-0.140874	2.414818	-1.041832
17	1	0	3.424386	-3.055158	-0.888746
18	1	0	3.347298	-1.486894	-1.704864
19	1	0	-2.328591	2.188946	0.894568
20	1	0	-1.512546	3.562209	1.656493
21	1	0	-1.973480	0.718273	2.405249
22	1	0	-1.092278	1.739491	3.545664
23	1	0	0.822537	0.196476	3.526881
24	1	0	-0.653248	-0.609127	4.029358
25	6	0	-1.061633	-2.110084	2.040262

26	1	0	-0.720536	-2.999451	1.498469
27	1	0	-1.332669	-2.436592	3.054404
28	6	0	-2.282157	-1.606995	1.309335
29	6	0	-3.574901	-1.936852	1.728768
30	6	0	-4.659510	-1.570444	0.929273
31	6	0	-3.102910	-0.609325	-0.624033
32	6	0	-4.419565	-0.910904	-0.276164
33	1	0	-5.216633	-0.627474	-0.953212
34	1	0	-3.721950	-2.474109	2.659837
35	1	0	-5.672385	-1.809607	1.238106
36	6	0	1.305499	-1.952928	2.392539
37	6	0	1.940232	-2.542675	1.138773
38	1	0	2.015595	-1.300350	2.904562
39	1	0	1.080010	-2.768021	3.095177
40	1	0	2.783324	-3.185110	1.436877
41	1	0	1.220431	-3.179214	0.614122
42	6	0	3.684081	0.623658	0.082344
43	6	0	3.567899	-0.763151	0.700457
44	1	0	3.876670	0.538561	-0.991752
45	1	0	4.551850	1.135625	0.528084
46	1	0	4.497308	-1.315683	0.500431
47	1	0	3.488108	-0.689247	1.785926
48	1	0	0.861099	3.437025	1.342923
49	1	0	0.829040	2.768967	2.965832
50	1	0	3.003707	2.403608	2.059641
51	1	0	2.215792	0.835517	2.201924
52	7	0	-2.057228	-0.927541	0.168894
53	6	0	-2.764149	0.046127	-1.954161
54	8	0	-3.690701	0.328255	-2.728681
55	8	0	-1.502996	0.227817	-2.156531
56	63	0	0.243108	0.075835	-0.509639
57	6	0	2.746548	2.717481	-0.524465
58	1	0	2.945796	2.465576	-1.568450
59	1	0	1.888344	3.384089	-0.493446
60	1	0	3.628911	3.222704	-0.102989
61	8	0	1.098221	0.934110	-2.776009

62	1	0	0.672967	1.800846	-2.554984
63	1	0	0.433617	0.489622	-3.338625

E(RTPSSh) = -1616.22126848

Zero-point correction= 0.517932 (Hartree/Particle)

Thermal correction to Energy= 0.549823

Thermal correction to Enthalpy= 0.550767

Thermal correction to Gibbs Free Energy= 0.457431

Sum of electronic and zero-point Energies= -1615.703337

Sum of electronic and thermal Energies= -1615.671446

Sum of electronic and thermal Enthalpies= -1615.670501

Sum of electronic and thermal Free Energies= -1615.763837

F8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.513434	0.823277	2.067921
2	7	0	-1.526424	2.178664	0.281744
3	7	0	-2.900136	-0.361005	-0.639215
4	6	0	-3.361277	-1.411865	0.312094
5	6	0	-2.734117	-1.378294	1.700616
6	7	0	-1.252489	-1.514993	1.714819
7	6	0	-0.735294	-1.130800	3.060479
8	6	0	0.574727	-0.357880	2.977255
9	6	0	-1.423109	3.125978	-0.853100
10	6	0	0.009524	3.164793	-1.411466
11	8	0	0.460674	4.220819	-1.865155
12	8	0	0.622781	2.015582	-1.395668
13	6	0	-0.848788	-2.914266	1.423213
14	6	0	-0.908354	-3.292875	-0.065092
15	8	0	-1.120710	-4.474881	-0.367427
16	8	0	-0.673921	-2.327086	-0.893595
17	1	0	-1.743201	4.135068	-0.560164
18	1	0	-2.080748	2.787766	-1.660751

19	1	0	0.196929	-3.028764	1.732624
20	1	0	-1.448887	-3.623349	2.010791
21	1	0	-4.453647	-1.343206	0.437645
22	1	0	-3.161549	-2.378032	-0.155042
23	1	0	-2.984602	-0.441387	2.201816
24	1	0	-3.194452	-2.184598	2.294339
25	6	0	1.858080	1.452401	2.065344
26	1	0	1.784362	2.417883	1.554190
27	1	0	2.194785	1.650897	3.093219
28	6	0	2.873968	0.618290	1.325317
29	6	0	4.216338	0.557534	1.712826
30	6	0	5.116177	-0.152986	0.916142
31	6	0	3.298793	-0.654910	-0.567645
32	6	0	4.653146	-0.760430	-0.251655
33	1	0	5.307710	-1.303405	-0.923286
34	1	0	4.543904	1.059445	2.617279
35	1	0	6.162253	-0.220612	1.198341
36	6	0	-0.481329	1.822572	2.543346
37	6	0	-0.870535	2.817655	1.456369
38	1	0	-1.369521	1.287821	2.882192
39	1	0	-0.092826	2.371072	3.414185
40	1	0	-1.533366	3.580399	1.892198
41	1	0	0.015052	3.345528	1.090770
42	6	0	-3.596005	0.940614	-0.427475
43	6	0	-2.947350	1.875328	0.592426
44	1	0	-3.626953	1.443067	-1.398113
45	1	0	-4.642595	0.774802	-0.129235
46	1	0	-3.536934	2.804822	0.630678
47	1	0	-2.986452	1.440786	1.592194
48	1	0	0.866771	-0.044638	3.991669
49	1	0	1.368168	-1.009665	2.596180
50	1	0	-1.495466	-0.540413	3.576341
51	1	0	-0.574132	-2.020009	3.683586
52	7	0	2.422658	0.000402	0.220036
53	6	0	2.739294	-1.210542	-1.863132
54	8	0	3.491186	-1.821928	-2.634407

55	8	0	1.485468	-0.952324	-2.046180
56	63	0	-0.133837	-0.080110	-0.448245
57	6	0	-3.271484	-0.849205	-1.996375
58	1	0	-4.354314	-1.038136	-2.060939
59	1	0	-2.984872	-0.107809	-2.741215
60	1	0	-2.725840	-1.773303	-2.194275
61	8	0	-0.611874	0.202474	-3.008554
62	1	0	0.135778	-0.419360	-3.179931
63	1	0	-0.156200	1.071932	-2.973980

E(RTPSSh) = -1616.21910111

Zero-point correction= 0.518197 (Hartree/Particle)

Thermal correction to Energy= 0.549919

Thermal correction to Enthalpy= 0.550863

Thermal correction to Gibbs Free Energy= 0.458096

Sum of electronic and zero-point Energies= -1615.700904

Sum of electronic and thermal Energies= -1615.669182

Sum of electronic and thermal Enthalpies= -1615.668238

Sum of electronic and thermal Free Energies= -1615.761005

F9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.089309	-0.581223	2.149111
2	7	0	1.242476	-2.388327	0.264089
3	6	0	2.585091	-2.382079	-0.380386
4	6	0	3.499976	-1.284031	0.144609
5	7	0	2.972670	0.082407	-0.125235
6	6	0	0.955822	1.645806	2.729188
7	6	0	-0.204242	0.677822	2.941096
8	6	0	0.438986	-3.453408	-0.385507
9	6	0	-0.145147	-3.029428	-1.741367
10	8	0	-0.415318	-3.903304	-2.573839
11	8	0	-0.372975	-1.760388	-1.869567

12	6	0	0.342719	3.166082	0.923111
13	6	0	0.329716	3.371355	-0.604186
14	8	0	-0.010603	4.467662	-1.061412
15	8	0	0.676696	2.326085	-1.291805
16	1	0	-0.419429	-3.682163	0.255257
17	1	0	1.017604	-4.380037	-0.501970
18	1	0	-0.690153	3.007693	1.256238
19	1	0	0.708913	4.079929	1.413437
20	1	0	3.080665	-3.354189	-0.227047
21	1	0	2.429319	-2.262109	-1.458677
22	1	0	4.496291	-1.408935	-0.303511
23	1	0	3.631411	-1.402231	1.223511
24	6	0	-1.323281	-1.368958	2.384065
25	1	0	-1.174284	-2.375074	1.982084
26	1	0	-1.523811	-1.478118	3.459751
27	6	0	-2.512203	-0.765380	1.677525
28	6	0	-3.808432	-0.849358	2.194195
29	6	0	-4.869217	-0.344893	1.439655
30	6	0	-3.281968	0.282451	-0.247402
31	6	0	-4.603581	0.224339	0.193882
32	1	0	-5.384908	0.623959	-0.441851
33	1	0	-3.976919	-1.302642	3.165461
34	1	0	-5.884744	-0.397198	1.819693
35	6	0	1.100190	-1.362009	2.570623
36	6	0	1.332092	-2.625633	1.735133
37	1	0	1.963623	-0.704274	2.477963
38	1	0	1.024144	-1.648388	3.631823
39	1	0	2.313165	-3.036960	2.005931
40	1	0	0.605436	-3.394496	2.008325
41	6	0	3.433160	1.022851	0.930504
42	6	0	2.581227	2.281589	1.013976
43	7	0	1.151651	1.982727	1.296498
44	1	0	2.626369	2.820284	0.066301
45	1	0	2.995979	2.944295	1.789197
46	1	0	3.414408	0.498691	1.889791
47	1	0	4.481164	1.313137	0.758168

48	1	0	-0.280205	0.444236	4.014548
49	1	0	-1.144084	1.154294	2.644525
50	1	0	0.764671	2.552114	3.321544
51	1	0	1.882314	1.218267	3.119532
52	7	0	-2.255534	-0.196512	0.485119
53	6	0	-2.919016	0.868695	-1.599672
54	8	0	-3.830936	1.272673	-2.337355
55	8	0	-1.654966	0.882866	-1.855886
56	63	0	0.160435	0.084655	-0.498171
57	6	0	3.483850	0.545387	-1.440875
58	1	0	3.200953	-0.167576	-2.216478
59	1	0	3.037953	1.510409	-1.687759
60	1	0	4.580401	0.639999	-1.417467
61	8	0	0.834359	0.396233	-2.988623
62	1	0	0.664544	1.362089	-2.881748
63	1	0	-0.006387	0.016410	-3.310004

E(RTPSSh) = -1616.21822373

Zero-point correction= 0.518258 (Hartree/Particle)

Thermal correction to Energy= 0.549950

Thermal correction to Enthalpy= 0.550894

Thermal correction to Gibbs Free Energy= 0.458348

Sum of electronic and zero-point Energies= -1615.699966

Sum of electronic and thermal Energies= -1615.668274

Sum of electronic and thermal Enthalpies= -1615.667330

Sum of electronic and thermal Free Energies= -1615.759876

F10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.835849	0.143236	0.045341
2	6	0	-3.524481	-1.107469	-0.773403
3	7	0	-2.308148	-1.830510	-0.314821
4	6	0	-2.453427	-2.302000	1.086229

5	6	0	-1.115188	-2.680494	1.706207
6	7	0	-0.183208	-1.520581	1.805962
7	6	0	-0.518313	-0.701898	2.994479
8	6	0	0.168613	0.659853	2.975471
9	6	0	-2.834936	2.173755	-0.849361
10	6	0	-1.524902	2.862454	-1.270245
11	8	0	-1.561315	4.053672	-1.603047
12	8	0	-0.477426	2.098868	-1.293776
13	6	0	1.197581	-2.049316	1.892911
14	6	0	1.640064	-2.644271	0.543807
15	8	0	2.549709	-3.483662	0.530946
16	8	0	1.018090	-2.167897	-0.487010
17	1	0	-3.547715	2.923857	-0.480240
18	1	0	-3.257660	1.737858	-1.761756
19	1	0	1.882449	-1.229649	2.133135
20	1	0	1.289292	-2.802590	2.687974
21	6	0	1.133752	2.373702	1.608082
22	1	0	0.873317	3.156464	0.888811
23	1	0	1.368006	2.859956	2.564977
24	6	0	2.343691	1.664954	1.045988
25	6	0	3.653227	1.924491	1.462002
26	6	0	4.710807	1.355063	0.746645
27	6	0	3.103028	0.383374	-0.744642
28	6	0	4.436204	0.593009	-0.391101
29	1	0	5.220885	0.176956	-1.012328
30	1	0	-0.626481	-3.446556	1.100963
31	1	0	-1.285722	-3.113840	2.702906
32	1	0	-2.915094	-1.510712	1.679696
33	1	0	-3.132295	-3.167690	1.130596
34	1	0	-0.222712	-1.221657	3.919546
35	1	0	-1.602996	-0.589640	3.034957
36	1	0	-0.145585	1.231701	3.860444
37	1	0	1.248215	0.509558	3.069027
38	1	0	-4.150396	-0.128820	1.055355
39	1	0	-4.696182	0.650422	-0.408294
40	1	0	-4.404063	-1.770718	-0.745155

41	1	0	-3.354345	-0.839915	-1.821378
42	1	0	3.837342	2.566653	2.316938
43	1	0	5.736028	1.531814	1.056916
44	6	0	-1.264373	2.333509	1.827054
45	6	0	-2.578859	1.624507	1.518974
46	7	0	-2.667874	1.074802	0.138587
47	7	0	-0.046274	1.473243	1.737292
48	1	0	-3.394538	2.343466	1.695363
49	1	0	-2.731057	0.799691	2.216477
50	1	0	-1.342376	2.770008	2.834046
51	1	0	-1.131965	3.165268	1.131938
52	7	0	2.086607	0.865980	-0.004444
53	6	0	2.698224	-0.282560	-2.051179
54	8	0	1.439962	-0.142896	-2.329999
55	8	0	3.562529	-0.824922	-2.750322
56	63	0	-0.233313	-0.113671	-0.528557
57	6	0	-2.106295	-3.001625	-1.204780
58	1	0	-2.945240	-3.708150	-1.113019
59	1	0	-2.031403	-2.652813	-2.235163
60	1	0	-1.174678	-3.505787	-0.943956
61	8	0	-0.957178	-0.699925	-2.960631
62	1	0	0.003500	-0.626088	-3.203048
63	1	0	-1.401915	0.012167	-3.454821

E(RTPSSh) = -1616.21848546

Zero-point correction= 0.518442 (Hartree/Particle)

Thermal correction to Energy= 0.550060

Thermal correction to Enthalpy= 0.551004

Thermal correction to Gibbs Free Energy= 0.459074

Sum of electronic and zero-point Energies= -1615.700043

Sum of electronic and thermal Energies= -1615.668425

Sum of electronic and thermal Enthalpies= -1615.667481

Sum of electronic and thermal Free Energies= -1615.759412

F11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.155695	-1.908883	1.452951
2	6	0	0.907667	-2.933843	1.249669
3	6	0	2.310847	-2.341207	1.196449
4	7	0	2.501479	-1.303792	0.142513
5	7	0	2.371507	1.724913	0.054796
6	6	0	2.222066	2.188238	1.466174
7	6	0	1.411196	1.273425	2.381305
8	7	0	0.006353	1.039232	1.944835
9	6	0	-0.647846	0.090161	2.889427
10	6	0	-0.068249	-1.317897	2.818309
11	6	0	2.830707	-1.960775	-1.153430
12	6	0	1.616439	-2.567790	-1.878281
13	8	0	1.767082	-3.601207	-2.537657
14	8	0	0.514534	-1.886235	-1.773336
15	6	0	-0.753397	2.318766	1.943867
16	6	0	-0.628818	3.097280	0.624418
17	8	0	-0.652992	4.334095	0.642048
18	8	0	-0.551333	2.353481	-0.435726
19	1	0	3.600276	-2.731103	-1.009657
20	1	0	3.242329	-1.199091	-1.825252
21	1	0	-1.815135	2.076439	2.061945
22	1	0	-0.460919	2.953419	2.790348
23	1	0	0.680844	-3.453154	0.316713
24	1	0	0.885484	-3.682304	2.056861
25	1	0	3.025679	-3.164978	1.054134
26	1	0	2.559804	-1.887685	2.159282
27	1	0	3.211742	2.333597	1.924797
28	1	0	1.747312	3.172863	1.437897
29	1	0	1.895880	0.301587	2.462988
30	1	0	1.414085	1.720599	3.388320
31	1	0	-1.711329	0.067643	2.639859
32	1	0	-0.559766	0.455924	3.924013
33	1	0	0.975432	-1.311426	3.132813

34	1	0	-0.600771	-1.950428	3.542647
35	6	0	-1.473626	-2.577313	1.294523
36	1	0	-1.373569	-3.311217	0.486855
37	1	0	-1.748285	-3.129382	2.203489
38	6	0	-2.580881	-1.641496	0.874912
39	6	0	-3.899469	-1.762101	1.325000
40	6	0	-3.205433	-0.057078	-0.708796
41	6	0	-4.885703	-0.962046	0.741422
42	1	0	-4.144976	-2.472452	2.107375
43	6	0	-4.540384	-0.110256	-0.309936
44	1	0	-5.913887	-1.027182	1.083517
45	1	0	-5.273925	0.491059	-0.834387
46	6	0	3.639372	-0.421051	0.534774
47	6	0	3.610622	0.928336	-0.163307
48	1	0	3.706685	0.795261	-1.245743
49	1	0	4.491910	1.501485	0.168236
50	1	0	4.599410	-0.909449	0.311789
51	1	0	3.612178	-0.278449	1.617170
52	7	0	-2.242297	-0.768460	-0.089372
53	6	0	-2.750201	0.695758	-1.946111
54	8	0	-1.535718	0.406529	-2.295030
55	8	0	-3.540793	1.443580	-2.534249
56	63	0	0.169666	0.070121	-0.538217
57	6	0	2.530244	2.943588	-0.784313
58	1	0	1.633529	3.561636	-0.707912
59	1	0	3.397776	3.533338	-0.451198
60	1	0	2.686790	2.650715	-1.823856
61	8	0	0.742979	1.476670	-2.665720
62	1	0	0.497490	2.288893	-2.169001
63	1	0	-0.141434	1.193675	-3.015502

E(RTPSSh) = -1616.21565263

Zero-point correction= 0.519308 (Hartree/Particle)

Thermal correction to Energy= 0.550646

Thermal correction to Enthalpy= 0.551590

Thermal correction to Gibbs Free Energy= 0.459874

Sum of electronic and zero-point Energies= -1615.696345

Sum of electronic and thermal Energies= -1615.665006

Sum of electronic and thermal Enthalpies= -1615.664062

Sum of electronic and thermal Free Energies= -1615.755779

F12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.316204	-1.285613	1.873131
2	6	0	1.465298	-2.240479	1.832523
3	6	0	2.813832	-1.575378	1.572775
4	7	0	2.850402	-0.739241	0.338547
5	7	0	1.980865	2.083730	-0.111755
6	7	0	-0.530164	1.578186	1.611476
7	6	0	-0.536638	0.829052	2.898978
8	6	0	0.513394	-0.274770	2.946483
9	6	0	3.309288	-1.569626	-0.804093
10	6	0	2.225937	-2.517030	-1.348424
11	8	0	2.568152	-3.603510	-1.829490
12	8	0	1.015137	-2.052618	-1.300658
13	6	0	-1.903185	2.043768	1.286418
14	6	0	-2.007017	2.481968	-0.185255
15	8	0	-2.904662	3.270825	-0.510082
16	8	0	-1.139403	1.939499	-0.977746
17	1	0	4.204692	-2.145560	-0.533199
18	1	0	3.587367	-0.898162	-1.625340
19	1	0	-2.600774	1.213524	1.438067
20	1	0	-2.219228	2.865402	1.943657
21	1	0	1.241558	-2.964537	1.046905
22	1	0	1.539939	-2.786939	2.785763
23	1	0	3.572777	-2.369063	1.521000
24	1	0	3.089495	-0.949270	2.423893
25	1	0	-1.530661	0.390605	3.026419
26	1	0	-0.379368	1.507104	3.749121

27	1	0	1.504747	0.161953	2.827084
28	1	0	0.489286	-0.756824	3.936182
29	6	0	-0.917834	-2.075008	2.152521
30	1	0	-0.721422	-3.112538	1.858585
31	1	0	-1.131160	-2.093118	3.229096
32	6	0	-2.140077	-1.644606	1.372473
33	6	0	-3.438409	-1.895188	1.833745
34	6	0	-4.517310	-1.628774	0.988602
35	6	0	-2.954973	-0.931988	-0.691875
36	6	0	-4.273940	-1.159860	-0.304938
37	1	0	-5.071682	-0.974128	-1.014506
38	1	0	-3.594609	-2.297799	2.829181
39	1	0	-5.532836	-1.805978	1.328771
40	6	0	3.776357	0.415959	0.513546
41	6	0	3.379164	1.619798	-0.334449
42	1	0	3.461932	1.376729	-1.399134
43	1	0	4.090220	2.437158	-0.133800
44	1	0	4.808031	0.135330	0.257186
45	1	0	3.789905	0.689461	1.570893
46	6	0	0.340489	2.796398	1.657159
47	6	0	1.803250	2.578811	1.278665
48	1	0	0.305223	3.236474	2.663969
49	1	0	-0.097300	3.531596	0.978176
50	1	0	2.258709	1.864793	1.965526
51	1	0	2.338710	3.532663	1.412072
52	7	0	-1.917039	-1.135889	0.148777
53	6	0	-2.587596	-0.513581	-2.107721
54	8	0	-3.491499	-0.274833	-2.918346
55	8	0	-1.312490	-0.494438	-2.330393
56	63	0	0.250247	0.040037	-0.520776
57	6	0	1.730467	3.189989	-1.070108
58	1	0	1.877287	2.815155	-2.084295
59	1	0	0.699355	3.529790	-0.983971
60	1	0	2.419204	4.027696	-0.882208
61	8	0	0.885865	0.689693	-2.965866
62	1	0	-0.019785	0.355872	-3.199912

63	1	0	1.501190	0.078379	-3.409023

E(RTPSSh) = -1616.21654685

Zero-point correction= 0.517964 (Hartree/Particle)

Thermal correction to Energy= 0.549717

Thermal correction to Enthalpy= 0.550661

Thermal correction to Gibbs Free Energy= 0.457616

Sum of electronic and zero-point Energies= -1615.698583

Sum of electronic and thermal Energies= -1615.666830

Sum of electronic and thermal Enthalpies= -1615.665886

Sum of electronic and thermal Free Energies= -1615.758931

F13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.343970	1.450668	1.712323
2	6	0	-0.702784	2.513139	1.820226
3	6	0	-2.120632	2.095232	1.421679
4	7	0	-2.245909	1.526228	0.049812
5	7	0	-2.455991	-1.378879	-0.738228
6	6	0	-2.770524	-2.210078	0.459714
7	6	0	-2.383464	-1.616229	1.813960
8	7	0	-0.950381	-1.233179	1.926140
9	6	0	-2.180042	2.621429	-0.956285
10	6	0	-0.749855	3.111725	-1.241803
11	8	0	-0.543993	4.316176	-1.425080
12	8	0	0.139225	2.164370	-1.319402
13	6	0	-0.108194	-2.448941	2.098807
14	6	0	0.231814	-3.166439	0.786978
15	8	0	0.345612	-4.399138	0.784369
16	8	0	0.432130	-2.379563	-0.221147
17	1	0	-2.811292	3.465028	-0.647397
18	1	0	-2.580542	2.232966	-1.900119
19	1	0	0.847532	-2.137029	2.535446

20	1	0	-0.583037	-3.145888	2.802612
21	1	0	-0.387066	3.344740	1.186745
22	1	0	-0.744862	2.899626	2.849381
23	1	0	-2.761688	2.984971	1.520922
24	1	0	-2.511687	1.355852	2.118214
25	1	0	-3.846507	-2.442311	0.484504
26	1	0	-2.248251	-3.161461	0.328850
27	1	0	-2.978815	-0.729692	2.029563
28	1	0	-2.640777	-2.358173	2.586368
29	6	0	1.671469	2.120865	1.580397
30	1	0	1.557990	2.928451	0.850397
31	1	0	1.982411	2.567055	2.534970
32	6	0	2.737442	1.194868	1.041237
33	6	0	4.071953	1.224284	1.457379
34	6	0	5.004982	0.437523	0.775180
35	6	0	3.243602	-0.296515	-0.676898
36	6	0	4.592554	-0.321966	-0.322075
37	1	0	5.284227	-0.915796	-0.908324
38	1	0	4.372224	1.853908	2.288312
39	1	0	6.045551	0.436395	1.084784
40	6	0	-3.560015	0.821063	-0.086933
41	6	0	-3.495815	-0.359070	-1.053068
42	1	0	-3.266516	0.007984	-2.058253
43	1	0	-4.491706	-0.828674	-1.094176
44	1	0	-4.328882	1.519055	-0.445147
45	1	0	-3.888372	0.494256	0.899656
46	6	0	0.424208	0.590195	2.929069
47	6	0	-0.751611	-0.357803	3.117690
48	1	0	0.524566	1.218708	3.827091
49	1	0	1.348492	0.008835	2.837908
50	1	0	-1.667921	0.199385	3.312116
51	1	0	-0.569372	-0.963415	4.016395
52	7	0	2.340511	0.417498	0.020063
53	6	0	2.708679	-0.979636	-1.926821
54	8	0	1.474178	-0.690201	-2.193508
55	8	0	3.466602	-1.694970	-2.594607

56	63	0	-0.123703	-0.093110	-0.456256
57	6	0	-2.385523	-2.308681	-1.899432
58	1	0	-3.324730	-2.870598	-2.010195
59	1	0	-2.203674	-1.733860	-2.808566
60	1	0	-1.559370	-3.004799	-1.741815
61	8	0	-0.851021	0.221232	-2.937452
62	1	0	-0.053965	-0.273564	-3.240146
63	1	0	-0.517413	1.144606	-2.866094

E(RTPSSh) = -1616.21840174

Zero-point correction= 0.519117 (Hartree/Particle)

Thermal correction to Energy= 0.550486

Thermal correction to Enthalpy= 0.551430

Thermal correction to Gibbs Free Energy= 0.460265

Sum of electronic and zero-point Energies= -1615.699285

Sum of electronic and thermal Energies= -1615.667916

Sum of electronic and thermal Enthalpies= -1615.666972

Sum of electronic and thermal Free Energies= -1615.758137

F14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.341428	-1.136538	1.911485
2	6	0	1.546035	-2.025220	1.932707
3	6	0	2.786273	-1.378800	1.316080
4	7	0	2.657580	-1.072734	-0.135450
5	6	0	3.742136	-0.155256	-0.587622
6	6	0	3.723118	1.194246	0.121208
7	7	0	2.378389	1.837079	0.069643
8	7	0	-0.362348	1.755595	1.491078
9	6	0	-0.512599	1.058056	2.796531
10	6	0	0.465025	-0.100955	2.977108
11	6	0	2.732704	-2.328519	-0.925294
12	6	0	1.378280	-3.044042	-1.065631

13	8	0	1.369455	-4.266807	-1.260045
14	8	0	0.343700	-2.268995	-1.015150
15	6	0	-1.654344	2.357388	1.070741
16	6	0	-1.609324	2.770451	-0.414860
17	8	0	-2.458922	3.570201	-0.830617
18	8	0	-0.676254	2.206361	-1.111788
19	1	0	3.481677	-3.014309	-0.507698
20	1	0	3.060191	-2.071550	-1.939469
21	1	0	-2.447916	1.613749	1.195084
22	1	0	-1.917818	3.227282	1.688483
23	1	0	1.295334	-2.941656	1.396118
24	1	0	1.788535	-2.310657	2.966989
25	1	0	3.642850	-2.049034	1.484802
26	1	0	3.010217	-0.450438	1.842980
27	1	0	4.731762	-0.617268	-0.448618
28	1	0	3.597029	-0.007028	-1.662578
29	1	0	4.476909	1.841037	-0.346872
30	1	0	4.027840	1.085264	1.164866
31	1	0	-1.536021	0.676869	2.853249
32	1	0	-0.388875	1.759525	3.634027
33	1	0	1.490872	0.268020	2.970670
34	1	0	0.298170	-0.557278	3.964664
35	6	0	-0.878689	-1.957700	2.146143
36	1	0	-0.691470	-2.947304	1.716115
37	1	0	-1.053784	-2.100706	3.220839
38	6	0	-2.132870	-1.453188	1.464474
39	6	0	-3.410357	-1.719104	1.972123
40	6	0	-4.524487	-1.414449	1.187092
41	6	0	-3.035097	-0.655805	-0.532828
42	6	0	-4.336822	-0.900889	-0.098603
43	1	0	-5.163931	-0.698032	-0.768745
44	1	0	-3.524021	-2.167116	2.953741
45	1	0	-5.524709	-1.603553	1.564250
46	6	0	0.624432	2.881026	1.546458
47	6	0	2.088555	2.499065	1.367704
48	1	0	0.518658	3.411848	2.504085

49	1	0	0.349810	3.585908	0.759342
50	1	0	2.406050	1.827277	2.168120
51	1	0	2.688775	3.417509	1.473498
52	7	0	-1.965789	-0.881803	0.259378
53	6	0	-2.724412	-0.219466	-1.959055
54	8	0	-3.663040	0.028968	-2.727412
55	8	0	-1.461435	-0.200181	-2.237860
56	63	0	0.256543	0.058200	-0.523633
57	6	0	2.362107	2.825641	-1.036848
58	1	0	2.643314	2.322742	-1.965016
59	1	0	1.355595	3.224763	-1.161861
60	1	0	3.073866	3.642271	-0.840817
61	8	0	0.987168	0.330248	-2.952096
62	1	0	0.037286	0.228290	-3.213775
63	1	0	1.463414	-0.367452	-3.436593

E(RTPSSh) = -1616.21500467

Zero-point correction= 0.517622 (Hartree/Particle)

Thermal correction to Energy= 0.549631

Thermal correction to Enthalpy= 0.550575

Thermal correction to Gibbs Free Energy= 0.457155

Sum of electronic and zero-point Energies= -1615.697382

Sum of electronic and thermal Energies= -1615.665374

Sum of electronic and thermal Enthalpies= -1615.664430

Sum of electronic and thermal Free Energies= -1615.757850

F15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.023580	1.223825	1.831209
2	6	0	-1.238906	2.089270	1.979626
3	6	0	-2.495295	1.550934	1.286291
4	7	0	-2.371254	1.472458	-0.193073
5	6	0	-3.581392	0.872700	-0.822671

6	6	0	-3.940551	-0.499492	-0.267663
7	7	0	-2.763837	-1.412237	-0.200740
8	7	0	-0.433398	-1.720630	1.638254
9	6	0	-2.167706	2.827679	-0.767152
10	6	0	-0.684073	3.194222	-0.915407
11	8	0	-0.343174	4.383650	-0.842015
12	8	0	0.097540	2.190576	-1.150457
13	6	0	0.880833	-2.405092	1.639395
14	6	0	1.218922	-2.929712	0.228582
15	8	0	2.067055	-3.824059	0.116005
16	8	0	0.580167	-2.348947	-0.737633
17	1	0	-2.699180	3.589503	-0.182879
18	1	0	-2.594750	2.835734	-1.775989
19	1	0	1.662992	-1.698554	1.935522
20	1	0	0.899841	-3.236056	2.359344
21	1	0	-0.998733	3.077530	1.578541
22	1	0	-1.472574	2.229087	3.043617
23	1	0	-3.341711	2.198207	1.566299
24	1	0	-2.717267	0.550405	1.660773
25	1	0	-4.450934	1.536788	-0.700475
26	1	0	-3.372006	0.801859	-1.894718
27	1	0	-4.733347	-0.931338	-0.892761
28	1	0	-4.364748	-0.393796	0.733876
29	6	0	1.197300	2.079265	1.803775
30	1	0	1.002332	2.926060	1.138204
31	1	0	1.423034	2.476495	2.802943
32	6	0	2.389201	1.343510	1.232503
33	6	0	3.698917	1.542735	1.680808
34	6	0	4.750684	0.957998	0.969805
35	6	0	3.142647	0.097330	-0.587808
36	6	0	4.474170	0.245879	-0.199433
37	1	0	5.256735	-0.173604	-0.821050
38	1	0	3.887982	2.151513	2.558765
39	1	0	5.774461	1.087147	1.307008
40	6	0	-0.669211	-0.989036	2.904081
41	6	0	0.152888	0.288878	2.984552

42	1	0	-0.076649	0.808051	3.926011
43	1	0	1.215260	0.031166	3.019363
44	1	0	-1.733976	-0.758612	2.976955
45	1	0	-0.422512	-1.618072	3.773650
46	6	0	-1.469876	-2.772601	1.448632
47	6	0	-2.822473	-2.207790	1.052300
48	1	0	-1.581336	-3.361905	2.371970
49	1	0	-1.110724	-3.448166	0.670455
50	1	0	-3.204900	-1.562435	1.847874
51	1	0	-3.538841	-3.038124	0.952763
52	7	0	2.128084	0.583362	0.153892
53	6	0	2.748823	-0.477187	-1.941715
54	8	0	3.608245	-1.030132	-2.639204
55	8	0	1.512945	-0.250624	-2.256664
56	63	0	-0.229938	-0.086713	-0.552331
57	6	0	-2.768618	-2.324760	-1.371205
58	1	0	-3.648587	-2.985813	-1.349895
59	1	0	-2.780709	-1.736031	-2.289756
60	1	0	-1.860100	-2.931934	-1.367837
61	8	0	-0.940710	-0.258729	-3.000709
62	1	0	0.018644	-0.333772	-3.240984
63	1	0	-1.257968	0.541876	-3.455874

E(RTPSSh) = -1616.21211723

Zero-point correction= 0.518278 (Hartree/Particle)

Thermal correction to Energy= 0.550056

Thermal correction to Enthalpy= 0.551000

Thermal correction to Gibbs Free Energy= 0.458384

Sum of electronic and zero-point Energies= -1615.693839

Sum of electronic and thermal Energies= -1615.662061

Sum of electronic and thermal Enthalpies= -1615.661117

Sum of electronic and thermal Free Energies= -1615.753734

F16

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.351691	1.178847	1.829161
2	6	0	-0.670741	2.255776	2.032910
3	6	0	-2.016698	1.998076	1.343565
4	7	0	-1.921189	1.897424	-0.136506
5	6	0	-3.234755	1.543386	-0.748697
6	6	0	-3.748694	0.165032	-0.350750
7	7	0	-2.780996	-0.924037	-0.658547
8	6	0	-3.000200	-2.075593	0.256046
9	6	0	-2.554043	-1.794308	1.688153
10	7	0	-1.118756	-1.421252	1.806965
11	6	0	-1.458665	3.194362	-0.698616
12	6	0	0.071442	3.268568	-0.828162
13	8	0	0.656421	4.338738	-0.618097
14	8	0	0.629601	2.154350	-1.195420
15	6	0	-0.288727	-2.653844	1.845933
16	6	0	-0.076998	-3.286517	0.463426
17	8	0	0.046972	-4.514581	0.375024
18	8	0	0.006203	-2.439923	-0.513323
19	1	0	-1.836324	4.038738	-0.108571
20	1	0	-1.868545	3.293316	-1.709792
21	1	0	0.705158	-2.388041	2.222663
22	1	0	-0.720493	-3.390421	2.537242
23	1	0	-0.250694	3.194229	1.662521
24	1	0	-0.859554	2.397430	3.105768
25	1	0	-2.701118	2.814335	1.625029
26	1	0	-2.454694	1.070696	1.712389
27	1	0	-3.997401	2.292758	-0.487112
28	1	0	-3.087981	1.580201	-1.831623
29	1	0	-4.698945	-0.013267	-0.875268
30	1	0	-3.981914	0.142903	0.715140
31	1	0	-4.067697	-2.348056	0.275468
32	1	0	-2.457761	-2.927751	-0.156265
33	1	0	-3.147710	-0.977416	2.107618
34	1	0	-2.774824	-2.679865	2.302925

35	6	0	1.717359	1.777892	1.784984
36	1	0	1.677561	2.664763	1.144088
37	1	0	2.036554	2.098907	2.786164
38	6	0	2.731085	0.835501	1.174349
39	6	0	4.066889	0.775732	1.584400
40	6	0	4.961287	-0.008851	0.850530
41	6	0	3.166720	-0.561104	-0.640974
42	6	0	4.512997	-0.673853	-0.293007
43	1	0	5.175900	-1.257213	-0.921430
44	1	0	4.397789	1.337440	2.451756
45	1	0	6.000770	-0.078822	1.155872
46	6	0	-0.892238	-0.647475	3.056898
47	6	0	0.361011	0.207010	2.963415
48	1	0	0.495905	0.748442	3.912124
49	1	0	1.241477	-0.429499	2.827755
50	1	0	-1.763084	-0.015041	3.245614
51	1	0	-0.800853	-1.315752	3.925677
52	7	0	2.297069	0.140847	0.109185
53	6	0	2.608512	-1.113969	-1.945040
54	8	0	3.327448	-1.836227	-2.648367
55	8	0	1.407137	-0.712156	-2.218883
56	63	0	-0.165284	-0.080259	-0.511278
57	6	0	-2.997842	-1.396073	-2.049852
58	1	0	-2.239116	-2.144944	-2.292560
59	1	0	-3.996210	-1.845638	-2.159951
60	1	0	-2.899751	-0.558257	-2.741192
61	8	0	-0.783593	0.664781	-2.905615
62	1	0	-0.123024	0.082536	-3.339681
63	1	0	-0.253002	1.468478	-2.673288

E(RTPSSh) = -1616.22090611

Zero-point correction= 0.519016 (Hartree/Particle)

Thermal correction to Energy= 0.550293

Thermal correction to Enthalpy= 0.551238

Thermal correction to Gibbs Free Energy= 0.460155

Sum of electronic and zero-point Energies= -1615.701890

Sum of electronic and thermal Energies= -1615.670613

Sum of electronic and thermal Enthalpies= -1615.669668

Sum of electronic and thermal Free Energies= -1615.760751

[Gd(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.163735	-1.542698	1.717260
2	6	0	1.351249	-2.447856	1.684179
3	6	0	2.649392	-1.727238	1.333307
4	7	0	2.655397	-1.104217	-0.018369
5	6	0	3.759740	-0.107360	-0.098939
6	6	0	3.436668	1.181482	0.649326
7	7	0	2.238757	1.871141	0.099242
8	6	0	1.707268	2.840073	1.095570
9	6	0	0.917829	2.179608	2.219645
10	7	0	-0.284377	1.415803	1.776576
11	6	0	-0.697273	0.507573	2.880688
12	6	0	0.197152	-0.724144	2.960290
13	6	0	2.834247	-2.149575	-1.058495
14	6	0	1.520856	-2.848064	-1.457243
15	8	0	1.573219	-4.005364	-1.892693
16	8	0	0.452438	-2.123252	-1.346677
17	6	0	-1.385550	2.354406	1.447015
18	6	0	-1.224941	2.998394	0.057928
19	8	0	-1.720915	4.114779	-0.144255
20	8	0	-0.606630	2.267906	-0.813210
21	1	0	3.577414	-2.896764	-0.749936
22	1	0	3.211598	-1.662193	-1.964529
23	1	0	-2.319805	1.781733	1.423520
24	1	0	-1.491197	3.133867	2.213861

25	1	0	1.152636	-3.232716	0.952310
26	1	0	1.483649	-2.940828	2.659232
27	1	0	3.474914	-2.451568	1.410973
28	1	0	2.853027	-0.947027	2.069342
29	1	0	4.696682	-0.528211	0.296073
30	1	0	3.926038	0.111493	-1.157037
31	1	0	4.311406	1.848537	0.606584
32	1	0	3.258902	0.971521	1.706512
33	1	0	2.534817	3.409021	1.547652
34	1	0	1.083832	3.556937	0.559559
35	1	0	1.567055	1.492035	2.765838
36	1	0	0.613525	2.958107	2.935695
37	1	0	-1.733526	0.210168	2.703811
38	1	0	-0.673193	1.031424	3.848066
39	1	0	1.231087	-0.422524	3.138927
40	1	0	-0.104935	-1.334819	3.824363
41	6	0	-1.066862	-2.375390	1.706365
42	1	0	-0.875719	-3.228922	1.047103
43	1	0	-1.280491	-2.775687	2.706964
44	6	0	-2.280296	-1.681105	1.133609
45	6	0	-3.581744	-1.964888	1.563382
46	6	0	-3.085312	-0.437168	-0.660379
47	6	0	-4.657974	-1.424257	0.856525
48	1	0	-3.742871	-2.603612	2.425557
49	6	0	-4.409552	-0.664497	-0.289146
50	1	0	-5.676007	-1.620653	1.178298
51	1	0	-5.207485	-0.267406	-0.905767
52	7	0	-2.046660	-0.891640	0.071317
53	6	0	-2.710371	0.213774	-1.981676
54	8	0	-3.584471	0.764776	-2.662578
55	8	0	-1.462136	0.054816	-2.284706
56	6	0	2.636400	2.644390	-1.101599
57	1	0	1.749623	3.134114	-1.510510
58	1	0	3.380875	3.413055	-0.844876
59	1	0	3.070756	1.980716	-1.852509
60	8	0	0.889378	0.740791	-2.947831

61	1	0	1.058172	1.694054	-3.048294
62	1	0	-0.080011	0.633957	-3.142409
63	64	0	0.251073	0.071702	-0.519891

E(RTPSSh) = -1616.81360478

Zero-point correction= 0.518687 (Hartree/Particle)

Thermal correction to Energy= 0.550167

Thermal correction to Enthalpy= 0.551111

Thermal correction to Gibbs Free Energy= 0.459188

Sum of electronic and zero-point Energies= -1616.294918

Sum of electronic and thermal Energies= -1616.263438

Sum of electronic and thermal Enthalpies= -1616.262494

Sum of electronic and thermal Free Energies= -1616.354416

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.241538	-0.913330	2.063705
2	6	0	0.865475	-1.836510	2.441551
3	6	0	1.238983	-2.800655	1.318447
4	7	0	1.806539	-2.115914	0.127160
5	6	0	3.236855	-1.789526	0.353810
6	6	0	3.717775	-0.663301	-0.553747
7	7	0	2.955106	0.600132	-0.379518
8	6	0	3.288087	1.201787	0.935549
9	6	0	2.321588	2.303162	1.337323
10	7	0	0.937155	1.792180	1.540967
11	6	0	0.813504	1.221984	2.904762
12	6	0	-0.333301	0.227396	3.022609
13	6	0	1.683495	-3.020842	-1.040091
14	6	0	0.249685	-3.065066	-1.591698
15	8	0	-0.106298	-4.050568	-2.248714
16	8	0	-0.468688	-2.013581	-1.344493
17	6	0	0.005428	2.927021	1.347293

18	6	0	-0.050301	3.341443	-0.137286
19	8	0	-0.469020	4.466689	-0.430567
20	8	0	0.345607	2.426980	-0.970025
21	1	0	2.022452	-4.036798	-0.793785
22	1	0	2.329366	-2.646378	-1.841902
23	1	0	-1.001715	2.621034	1.653976
24	1	0	0.287735	3.792514	1.963483
25	6	0	-1.523161	-1.657842	2.147662
26	1	0	-1.389568	-2.627857	1.658295
27	1	0	-1.785761	-1.857627	3.196596
28	6	0	-2.651828	-0.951169	1.439268
29	6	0	-3.978691	-1.056047	1.870588
30	6	0	-3.299819	0.198547	-0.468546
31	6	0	-4.988584	-0.492770	1.088967
32	1	0	-4.209700	-1.576148	2.794401
33	6	0	-4.646088	0.132460	-0.110836
34	1	0	-6.025491	-0.556685	1.403990
35	1	0	-5.387149	0.557877	-0.777525
36	1	0	2.287835	3.071937	0.563561
37	1	0	2.682289	2.787642	2.256825
38	1	0	3.274859	0.415224	1.692902
39	1	0	4.313061	1.606332	0.917849
40	1	0	0.664669	2.018338	3.649211
41	1	0	1.760807	0.738272	3.156612
42	1	0	-0.374497	-0.150722	4.055533
43	1	0	-1.285703	0.730314	2.825841
44	1	0	0.588277	-2.414293	3.336199
45	1	0	1.733234	-1.232889	2.715333
46	1	0	0.358185	-3.358747	0.989218
47	1	0	1.953036	-3.541028	1.709920
48	1	0	3.367322	-1.520768	1.404376
49	1	0	3.865135	-2.676717	0.183641
50	1	0	4.791810	-0.494085	-0.372519
51	1	0	3.614009	-0.958418	-1.602607
52	7	0	-2.319970	-0.305877	0.308054
53	6	0	-2.860112	0.761363	-1.805989

54	8	0	-3.709160	1.240004	-2.571055
55	8	0	-1.593064	0.646402	-2.030665
56	6	0	3.381194	1.527692	-1.454441
57	1	0	2.808161	2.453873	-1.393920
58	1	0	4.454895	1.757763	-1.370887
59	1	0	3.191888	1.062202	-2.423429
60	8	0	0.819114	0.668553	-2.903058
61	1	0	0.878744	1.615076	-2.637159
62	1	0	-0.136612	0.597378	-3.140719
63	64	0	0.172474	0.067070	-0.463726

E(RTPSSh) = -1616.81625359

Zero-point correction= 0.518661 (Hartree/Particle)

Thermal correction to Energy= 0.550217

Thermal correction to Enthalpy= 0.551162

Thermal correction to Gibbs Free Energy= 0.458665

Sum of electronic and zero-point Energies= -1616.297592

Sum of electronic and thermal Energies= -1616.266036

Sum of electronic and thermal Enthalpies= -1616.265092

Sum of electronic and thermal Free Energies= -1616.357589

[Ho(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.078545	-1.433247	1.814622
2	6	0	1.214216	-2.402994	1.801164
3	6	0	2.534872	-1.772413	1.365882
4	7	0	2.525137	-1.210650	-0.015547
5	6	0	3.697450	-0.306906	-0.182925
6	6	0	3.499713	1.032445	0.518056
7	7	0	2.324745	1.766880	-0.020076

8	6	0	1.870447	2.797851	0.951165
9	6	0	1.076495	2.222692	2.115889
10	7	0	-0.181673	1.523339	1.727873
11	6	0	-0.641810	0.709633	2.884790
12	6	0	0.174550	-0.569821	3.022995
13	6	0	2.599238	-2.312307	-1.009959
14	6	0	1.236779	-2.965893	-1.292561
15	8	0	1.209766	-4.141448	-1.681020
16	8	0	0.213506	-2.188183	-1.139908
17	6	0	-1.216310	2.520440	1.356342
18	6	0	-1.047589	3.044550	-0.080230
19	8	0	-1.487501	4.166974	-0.362083
20	8	0	-0.483184	2.215976	-0.898407
21	1	0	3.328480	-3.074516	-0.704447
22	1	0	2.939522	-1.884161	-1.958837
23	1	0	-2.194364	2.028103	1.402593
24	1	0	-1.234929	3.361225	2.063116
25	1	0	0.949883	-3.219863	1.128487
26	1	0	1.357071	-2.840163	2.800795
27	1	0	3.323594	-2.535702	1.448579
28	1	0	2.806365	-0.969941	2.055477
29	1	0	4.615315	-0.783555	0.192024
30	1	0	3.831826	-0.146422	-1.255967
31	1	0	4.413515	1.635834	0.407165
32	1	0	3.353779	0.884391	1.590506
33	1	0	2.738606	3.337793	1.360764
34	1	0	1.274325	3.528894	0.402606
35	1	0	1.698235	1.513613	2.666749
36	1	0	0.839990	3.040742	2.813605
37	1	0	-1.696093	0.467089	2.729492
38	1	0	-0.576485	1.284750	3.820479
39	1	0	1.227077	-0.328241	3.185004
40	1	0	-0.161374	-1.121340	3.913466
41	6	0	-1.205590	-2.181125	1.844342
42	1	0	-1.067555	-3.086328	1.243790
43	1	0	-1.453294	-2.498835	2.866259

44	6	0	-2.367672	-1.450943	1.209351
45	6	0	-3.692437	-1.643861	1.617731
46	6	0	-3.064007	-0.298812	-0.691439
47	6	0	-4.721412	-1.104804	0.842130
48	1	0	-3.908499	-2.215537	2.514248
49	6	0	-4.407268	-0.445474	-0.349162
50	1	0	-5.755978	-1.231298	1.145803
51	1	0	-5.169361	-0.067523	-1.020813
52	7	0	-2.071475	-0.738770	0.109157
53	6	0	-2.616456	0.219604	-2.050128
54	8	0	-3.454325	0.699154	-2.824732
55	8	0	-1.357146	0.029700	-2.276772
56	6	0	2.726929	2.481377	-1.255361
57	1	0	1.839846	2.931214	-1.707905
58	1	0	3.456599	3.273503	-1.030002
59	1	0	3.194096	1.787216	-1.957982
60	8	0	1.137120	0.243250	-2.779493
61	1	0	1.460546	1.117565	-3.059554
62	1	0	0.203021	0.200614	-3.111042
63	67	0	0.231531	0.039033	-0.466654

E(RTPSSh) = -1618.57146498

Zero-point correction= 0.518374 (Hartree/Particle)

Thermal correction to Energy= 0.549963

Thermal correction to Enthalpy= 0.550908

Thermal correction to Gibbs Free Energy= 0.458674

Sum of electronic and zero-point Energies= -1618.053091

Sum of electronic and thermal Energies= -1618.021502

Sum of electronic and thermal Enthalpies= -1618.020557

Sum of electronic and thermal Free Energies= -1618.112791

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.272314	-0.898572	2.071277
2	6	0	0.817164	-1.837523	2.456867
3	6	0	1.161396	-2.810751	1.333220
4	7	0	1.734071	-2.134786	0.139221
5	6	0	3.174712	-1.848492	0.359731
6	6	0	3.672999	-0.734089	-0.550045
7	7	0	2.929947	0.540546	-0.372616
8	6	0	3.274029	1.133967	0.944771
9	6	0	2.335556	2.260285	1.341964
10	7	0	0.937911	1.781769	1.540352
11	6	0	0.795634	1.230788	2.909729
12	6	0	-0.359394	0.247026	3.024993
13	6	0	1.589208	-3.040095	-1.026497
14	6	0	0.165194	-3.019949	-1.597194
15	8	0	-0.244840	-3.999252	-2.230887
16	8	0	-0.485266	-1.916746	-1.393329
17	6	0	0.032467	2.933941	1.313780
18	6	0	0.035514	3.320211	-0.178939
19	8	0	-0.308546	4.459196	-0.511480
20	8	0	0.402131	2.363486	-0.977657
21	1	0	1.882868	-4.067411	-0.771222
22	1	0	2.259561	-2.694647	-1.821078
23	1	0	-0.988083	2.652052	1.598428
24	1	0	0.319181	3.801163	1.924947
25	6	0	-1.564411	-1.624355	2.158122
26	1	0	-1.445722	-2.604791	1.686456
27	1	0	-1.836391	-1.803149	3.208380
28	6	0	-2.671606	-0.906102	1.431659
29	6	0	-4.005493	-0.987749	1.845158
30	6	0	-3.270554	0.253479	-0.483202
31	6	0	-4.994356	-0.407310	1.049696
32	1	0	-4.257197	-1.501899	2.766973
33	6	0	-4.622870	0.210322	-0.145267
34	1	0	-6.036420	-0.451282	1.350924
35	1	0	-5.346048	0.649038	-0.822818
36	1	0	2.326321	3.029803	0.568396

37	1	0	2.704445	2.735330	2.262795
38	1	0	3.236152	0.348700	1.702765
39	1	0	4.309675	1.509814	0.930361
40	1	0	0.646810	2.036903	3.643239
41	1	0	1.736286	0.741337	3.175980
42	1	0	-0.410847	-0.126437	4.059052
43	1	0	-1.305678	0.757931	2.819528
44	1	0	0.531535	-2.404967	3.355327
45	1	0	1.697693	-1.249412	2.724174
46	1	0	0.265580	-3.347522	1.008889
47	1	0	1.861580	-3.568261	1.716013
48	1	0	3.319838	-1.585098	1.409688
49	1	0	3.777205	-2.751860	0.183347
50	1	0	4.750063	-0.581334	-0.373998
51	1	0	3.558170	-1.027362	-1.598214
52	7	0	-2.309734	-0.267961	0.305894
53	6	0	-2.799344	0.810629	-1.810680
54	8	0	-3.631522	1.283055	-2.599400
55	8	0	-1.528088	0.700384	-2.001172
56	6	0	3.386498	1.463925	-1.440585
57	1	0	2.824772	2.397251	-1.390709
58	1	0	4.461276	1.678513	-1.336371
59	1	0	3.211761	0.999976	-2.412758
60	8	0	0.891130	0.481028	-2.806517
61	1	0	0.948466	1.447676	-2.627682
62	1	0	-0.047805	0.394472	-3.095907
63	67	0	0.182563	0.068363	-0.434238

E(RTPSSh) = -1618.57152902

Zero-point correction= 0.519290 (Hartree/Particle)

Thermal correction to Energy= 0.550626

Thermal correction to Enthalpy= 0.551571

Thermal correction to Gibbs Free Energy= 0.460033

Sum of electronic and zero-point Energies= -1618.052239

Sum of electronic and thermal Energies= -1618.020903

Sum of electronic and thermal Enthalpies= -1618.019959

Sum of electronic and thermal Free Energies= -1618.111496

[Yb(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.076577	-1.430122	1.818148
2	6	0	1.208024	-2.403527	1.800700
3	6	0	2.525317	-1.772335	1.357578
4	7	0	2.499842	-1.201905	-0.020234
5	6	0	3.676169	-0.305289	-0.196165
6	6	0	3.489363	1.032363	0.509465
7	7	0	2.311462	1.765896	-0.021356
8	6	0	1.860011	2.793986	0.953045
9	6	0	1.071822	2.213688	2.117815
10	7	0	-0.182760	1.508488	1.729124
11	6	0	-0.641809	0.704515	2.892690
12	6	0	0.175020	-0.573761	3.030563
13	6	0	2.559884	-2.299104	-1.020522
14	6	0	1.192026	-2.944598	-1.286369
15	8	0	1.150945	-4.115560	-1.687140
16	8	0	0.175594	-2.163750	-1.105511
17	6	0	-1.217164	2.502013	1.348490
18	6	0	-1.042828	3.007560	-0.093021
19	8	0	-1.484189	4.123950	-0.395202
20	8	0	-0.467725	2.169877	-0.894589
21	1	0	3.290697	-3.064639	-0.727487
22	1	0	2.887275	-1.866480	-1.971388
23	1	0	-2.195942	2.011798	1.400151
24	1	0	-1.234898	3.350913	2.045467
25	1	0	0.938889	-3.220355	1.130002
26	1	0	1.355250	-2.840116	2.799849

27	1	0	3.314845	-2.535954	1.427134
28	1	0	2.803446	-0.973849	2.049302
29	1	0	4.594173	-0.789023	0.168869
30	1	0	3.800780	-0.142537	-1.269910
31	1	0	4.403386	1.634339	0.393042
32	1	0	3.350478	0.882675	1.582656
33	1	0	2.728859	3.334413	1.360655
34	1	0	1.260775	3.526148	0.409167
35	1	0	1.698005	1.506826	2.666473
36	1	0	0.831407	3.029042	2.817296
37	1	0	-1.696945	0.462259	2.743020
38	1	0	-0.572126	1.285233	3.824445
39	1	0	1.227706	-0.332354	3.192071
40	1	0	-0.160132	-1.128850	3.919022
41	6	0	-1.212129	-2.168729	1.843608
42	1	0	-1.080629	-3.072474	1.239428
43	1	0	-1.465151	-2.487713	2.863791
44	6	0	-2.364473	-1.425016	1.207513
45	6	0	-3.693493	-1.609950	1.605647
46	6	0	-3.038807	-0.265131	-0.695782
47	6	0	-4.712954	-1.060099	0.825252
48	1	0	-3.919732	-2.184108	2.498052
49	6	0	-4.385357	-0.402459	-0.363492
50	1	0	-5.750527	-1.179242	1.121558
51	1	0	-5.139734	-0.020789	-1.041719
52	7	0	-2.054894	-0.709264	0.113381
53	6	0	-2.574954	0.233972	-2.055719
54	8	0	-3.400439	0.714707	-2.843199
55	8	0	-1.317659	0.021275	-2.268540
56	6	0	2.709561	2.486773	-1.254109
57	1	0	1.818774	2.924171	-1.711928
58	1	0	3.426340	3.289392	-1.024551
59	1	0	3.193924	1.800991	-1.953549
60	8	0	1.183930	0.192994	-2.694008
61	1	0	1.501647	1.073792	-2.960792
62	1	0	0.262932	0.139164	-3.060064

63	70	0	0.225023	0.029121	-0.447445

E(RTPSSh) = -1620.31668239

Zero-point correction= 0.518731 (Hartree/Particle)

Thermal correction to Energy= 0.550192

Thermal correction to Enthalpy= 0.551137

Thermal correction to Gibbs Free Energy= 0.459349

Sum of electronic and zero-point Energies= -1619.797952

Sum of electronic and thermal Energies= -1619.766490

Sum of electronic and thermal Enthalpies= -1619.765546

Sum of electronic and thermal Free Energies= -1619.857334

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.277829	-0.809396	2.095250
2	6	0	0.809109	-1.744758	2.498714
3	6	0	1.148466	-2.740173	1.392873
4	7	0	1.718109	-2.081366	0.185062
5	6	0	3.165607	-1.820713	0.394810
6	6	0	3.679761	-0.736276	-0.539936
7	7	0	2.937808	0.540540	-0.396015
8	6	0	3.278032	1.166020	0.905902
9	6	0	2.339246	2.304461	1.265100
10	7	0	0.942855	1.830605	1.480515
11	6	0	0.799808	1.338151	2.871305
12	6	0	-0.355384	0.359773	3.022279
13	6	0	1.557275	-2.995440	-0.972263
14	6	0	0.107550	-3.029787	-1.467789
15	8	0	-0.291279	-4.009302	-2.108529
16	8	0	-0.580978	-1.968194	-1.186928
17	6	0	0.034042	2.966031	1.193501
18	6	0	0.045213	3.260899	-0.320972
19	8	0	-0.273654	4.385112	-0.723614

20	8	0	0.393781	2.251257	-1.059176
21	1	0	1.900586	-4.010181	-0.728082
22	1	0	2.176230	-2.625850	-1.796605
23	1	0	-0.986282	2.698579	1.492445
24	1	0	0.319582	3.866957	1.754031
25	6	0	-1.576954	-1.522909	2.202540
26	1	0	-1.466184	-2.513020	1.749938
27	1	0	-1.848296	-1.674222	3.256823
28	6	0	-2.674997	-0.810242	1.456224
29	6	0	-4.011910	-0.846021	1.865405
30	6	0	-3.240484	0.277210	-0.513232
31	6	0	-4.983206	-0.275843	1.040104
32	1	0	-4.280648	-1.315732	2.805901
33	6	0	-4.594849	0.278477	-0.180615
34	1	0	-6.027070	-0.281862	1.338332
35	1	0	-5.307034	0.699945	-0.880466
36	1	0	2.329551	3.047353	0.465650
37	1	0	2.706810	2.811764	2.168910
38	1	0	3.232237	0.402064	1.685181
39	1	0	4.315246	1.538200	0.888510
40	1	0	0.650208	2.172904	3.571817
41	1	0	1.740262	0.859501	3.157591
42	1	0	-0.399993	0.011237	4.064962
43	1	0	-1.302395	0.867052	2.811255
44	1	0	0.522459	-2.292744	3.408491
45	1	0	1.691373	-1.153073	2.752595
46	1	0	0.251274	-3.282277	1.083367
47	1	0	1.851870	-3.489174	1.785291
48	1	0	3.319515	-1.538419	1.438571
49	1	0	3.745960	-2.741386	0.235447
50	1	0	4.756726	-0.586325	-0.359797
51	1	0	3.569755	-1.055598	-1.580758
52	7	0	-2.298165	-0.225593	0.307617
53	6	0	-2.742206	0.745417	-1.865523
54	8	0	-3.553349	1.198652	-2.687199
55	8	0	-1.474348	0.581201	-2.036904

56	6	0	3.391216	1.439542	-1.484273
57	1	0	2.796692	2.353757	-1.486606
58	1	0	4.455468	1.695066	-1.364010
59	1	0	3.266557	0.932188	-2.443167
60	8	0	0.951641	0.107669	-2.710916
61	1	0	1.102486	1.077291	-2.717170
62	1	0	0.019465	0.048002	-3.031302
63	70	0	0.161595	0.037720	-0.395899

E(RTPSSh) = -1620.31474557

Zero-point correction= 0.519170 (Hartree/Particle)

Thermal correction to Energy= 0.550552

Thermal correction to Enthalpy= 0.551496

Thermal correction to Gibbs Free Energy= 0.459912

Sum of electronic and zero-point Energies= -1619.795576

Sum of electronic and thermal Energies= -1619.764194

Sum of electronic and thermal Enthalpies= -1619.763250

Sum of electronic and thermal Free Energies= -1619.854833

[Lu(1,7-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.117387	-1.427887	1.815000
2	6	0	1.272030	-2.373333	1.801108
3	6	0	2.572914	-1.704229	1.365714
4	7	0	2.527698	-1.124269	-0.007504
5	6	0	3.676077	-0.191525	-0.179469
6	6	0	3.438396	1.138196	0.523764
7	7	0	2.235870	1.826936	-0.015449
8	6	0	1.749208	2.844191	0.955217
9	6	0	0.980097	2.245008	2.123342

10	7	0	-0.241809	1.485252	1.733158
11	6	0	-0.672738	0.670991	2.899903
12	6	0	0.185211	-0.579511	3.035049
13	6	0	2.623458	-2.214839	-1.014165
14	6	0	1.276991	-2.900646	-1.285405
15	8	0	1.271671	-4.066362	-1.702490
16	8	0	0.236409	-2.155530	-1.090473
17	6	0	-1.314583	2.433785	1.344161
18	6	0	-1.147520	2.946161	-0.095329
19	8	0	-1.626099	4.045784	-0.402085
20	8	0	-0.535380	2.129796	-0.891463
21	1	0	3.377284	-2.958479	-0.723493
22	1	0	2.938028	-1.767595	-1.962325
23	1	0	-2.271270	1.901033	1.385827
24	1	0	-1.375113	3.280643	2.041253
25	1	0	1.027703	-3.193594	1.125250
26	1	0	1.424544	-2.809929	2.799299
27	1	0	3.382509	-2.447074	1.426881
28	1	0	2.831065	-0.905361	2.064592
29	1	0	4.606728	-0.645227	0.191589
30	1	0	3.801714	-0.026620	-1.252652
31	1	0	4.329644	1.774278	0.413414
32	1	0	3.297823	0.982513	1.595999
33	1	0	2.600188	3.414696	1.359043
34	1	0	1.125705	3.552907	0.408037
35	1	0	1.631057	1.569375	2.682614
36	1	0	0.703274	3.056753	2.813181
37	1	0	-1.719761	0.394459	2.753174
38	1	0	-0.619896	1.255771	3.830042
39	1	0	1.229041	-0.304962	3.202130
40	1	0	-0.134834	-1.152572	3.917617
41	6	0	-1.154045	-2.198592	1.827982
42	1	0	-0.998028	-3.091613	1.214001
43	1	0	-1.402721	-2.533874	2.843845
44	6	0	-2.321012	-1.475490	1.194393
45	6	0	-3.647900	-1.682731	1.588917

46	6	0	-3.010158	-0.319170	-0.706860
47	6	0	-4.673910	-1.143150	0.809555
48	1	0	-3.867636	-2.264318	2.478089
49	6	0	-4.354878	-0.475405	-0.376120
50	1	0	-5.710070	-1.277856	1.104153
51	1	0	-5.114304	-0.100826	-1.052746
52	7	0	-2.021899	-0.751551	0.103139
53	6	0	-2.547570	0.185225	-2.065333
54	8	0	-3.372505	0.670572	-2.850417
55	8	0	-1.290847	-0.030812	-2.278299
56	6	0	2.617026	2.562248	-1.245422
57	1	0	1.713797	2.963526	-1.711596
58	1	0	3.298731	3.392815	-1.008963
59	1	0	3.137113	1.897038	-1.939072
60	8	0	1.204836	0.204172	-2.664636
61	1	0	1.508372	1.088567	-2.935823
62	1	0	0.289622	0.127731	-3.041716
63	71	0	0.228897	0.025132	-0.442072

E(RTPSSh) = -1620.87040542

Zero-point correction= 0.519038 (Hartree/Particle)

Thermal correction to Energy= 0.550326

Thermal correction to Enthalpy= 0.551270

Thermal correction to Gibbs Free Energy= 0.460192

Sum of electronic and zero-point Energies= -1620.351367

Sum of electronic and thermal Energies= -1620.320079

Sum of electronic and thermal Enthalpies= -1620.319135

Sum of electronic and thermal Free Energies= -1620.410213

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.140435	-0.799996	2.126582
2	6	0	1.067434	-1.546225	2.574235

3	6	0	1.621554	-2.465812	1.493510
4	7	0	2.068331	-1.724721	0.279457
5	6	0	3.431903	-1.176100	0.494620
6	6	0	3.748293	-0.052714	-0.484263
7	7	0	2.757185	1.052547	-0.418156
8	6	0	2.950587	1.813820	0.843466
9	6	0	1.773960	2.724177	1.150565
10	7	0	0.533968	1.945120	1.423469
11	6	0	0.536377	1.503599	2.837042
12	6	0	-0.411357	0.337079	3.052748
13	6	0	2.083458	-2.675767	-0.859621
14	6	0	0.655080	-3.031321	-1.294480
15	8	0	0.463145	-4.061140	-1.951802
16	8	0	-0.247544	-2.170443	-0.938318
17	6	0	-0.630357	2.812536	1.132594
18	6	0	-0.726701	3.057042	-0.384287
19	8	0	-1.346080	4.042225	-0.802331
20	8	0	-0.133010	2.157974	-1.106321
21	1	0	2.642721	-3.587788	-0.608309
22	1	0	2.580734	-2.200293	-1.710218
23	1	0	-1.546817	2.312463	1.465539
24	1	0	-0.565037	3.771798	1.665152
25	6	0	-1.329742	-1.683545	2.176123
26	1	0	-1.084852	-2.623110	1.670858
27	1	0	-1.602048	-1.918989	3.214583
28	6	0	-2.490353	-1.065144	1.435279
29	6	0	-3.820643	-1.232029	1.831501
30	6	0	-3.147058	-0.056576	-0.552638
31	6	0	-4.836281	-0.748149	1.003834
32	1	0	-4.049968	-1.737991	2.763410
33	6	0	-4.496444	-0.172073	-0.221569
34	1	0	-5.876408	-0.851356	1.296982
35	1	0	-5.242345	0.161613	-0.933628
36	1	0	1.582867	3.386630	0.304623
37	1	0	2.015456	3.361486	2.013490
38	1	0	3.087233	1.103296	1.662085

39	1	0	3.873643	2.411636	0.785491
40	1	0	0.255670	2.328524	3.508495
41	1	0	1.558085	1.219625	3.103037
42	1	0	-0.354120	-0.001150	4.097831
43	1	0	-1.442207	0.658434	2.876798
44	1	0	0.839864	-2.137535	3.473573
45	1	0	1.824288	-0.813148	2.862332
46	1	0	0.857293	-3.181618	1.183289
47	1	0	2.455839	-3.048219	1.910739
48	1	0	3.499648	-0.819371	1.525372
49	1	0	4.186192	-1.969517	0.388838
50	1	0	4.766100	0.320220	-0.289196
51	1	0	3.737554	-0.437218	-1.508246
52	7	0	-2.165222	-0.434679	0.291667
53	6	0	-2.688977	0.333453	-1.946499
54	8	0	-3.516549	0.758308	-2.765148
55	8	0	-1.436074	0.100895	-2.147741
56	6	0	3.008313	1.971427	-1.555726
57	1	0	2.178652	2.672424	-1.656683
58	1	0	3.947641	2.526724	-1.415176
59	1	0	3.108963	1.393671	-2.478154
60	8	0	1.028098	-0.195234	-2.672151
61	1	0	1.362950	0.660995	-2.995316
62	1	0	0.088730	-0.214085	-2.991507
63	71	0	0.192208	0.000524	-0.399934

E(RTPSSh) = -1620.86767470

Zero-point correction= 0.518831 (Hartree/Particle)

Thermal correction to Energy= 0.550378

Thermal correction to Enthalpy= 0.551322

Thermal correction to Gibbs Free Energy= 0.459137

Sum of electronic and zero-point Energies= -1620.348844

Sum of electronic and thermal Energies= -1620.317296

Sum of electronic and thermal Enthalpies= -1620.316352

Sum of electronic and thermal Free Energies= -1620.408538

Complejos de 1,4-H_3Medo2ampa

Las geometrías optimizadas en disolución se corresponden con las siguientes conformaciones:

- F1: Δ(λλλλ)
- F2: Δ(δδδδ)
- F3: Δ(λλλδ)
- F4: Δ(λλδδ)
- F5: Δ(λδλδ)
- F6: Δ(δλλδ)
- F7: Δ(λδδδ)
- F8: Δ(δλδδ)
- F9: Δ(δδλδ)
- F10: Δ(δδδλ)
- F11: Δ(λλδλ)
- F12: Δ(λδδλ)
- F13: Δ(δλδλ)
- F14: Δ(λδλλ)
- F15: Δ(δδλλ)
- F16: Δ(δλλλ)

[La(1,4-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.725472	1.716097	1.312034
2	6	0	-0.286874	2.807165	1.432340
3	6	0	-1.715586	2.296748	1.590663
4	7	0	-2.204490	1.500411	0.439444
5	6	0	-3.425689	0.750829	0.833467
6	6	0	-3.114661	-0.460241	1.707127
7	7	0	-2.217567	-1.457981	1.064106
8	6	0	-1.591354	-2.306942	2.119600
9	6	0	-0.476167	-1.589053	2.879605
10	7	0	0.706851	-1.274032	2.034895
11	6	0	1.559256	-0.255658	2.703958
12	6	0	0.984081	1.159151	2.672002
13	6	0	-2.511795	2.383245	-0.708553
14	6	0	-1.279467	2.817735	-1.519359
15	8	0	-1.292632	3.910763	-2.094955

16	8	0	-0.317854	1.939435	-1.590486
17	6	0	-2.996488	-2.308648	0.127388
18	6	0	-3.263363	-1.674848	-1.253294
19	8	0	-4.253317	-2.049829	-1.890818
20	8	0	-2.368479	-0.826618	-1.664053
21	1	0	-3.077813	3.272226	-0.395870
22	1	0	-3.135569	1.809156	-1.402550
23	1	0	-3.949359	-2.622765	0.574513
24	1	0	-2.411412	-3.215724	-0.066916
25	1	0	-0.211259	3.435544	0.543512
26	1	0	-0.051583	3.448590	2.295462
27	1	0	-2.373088	3.165904	1.755849
28	1	0	-1.790555	1.677031	2.487213
29	1	0	-4.125539	1.401924	1.381419
30	1	0	-3.929966	0.434676	-0.080816
31	1	0	-4.062972	-0.942453	1.990492
32	1	0	-2.645451	-0.133754	2.637316
33	1	0	-2.348998	-2.646787	2.841955
34	1	0	-1.193237	-3.200184	1.630792
35	1	0	-0.853738	-0.656463	3.305341
36	1	0	-0.170451	-2.219279	3.729808
37	1	0	2.535520	-0.277903	2.217135
38	1	0	1.721344	-0.528855	3.759576
39	1	0	0.038899	1.179256	3.218902
40	1	0	1.671332	1.820587	3.221671
41	6	0	1.958197	2.319380	0.738028
42	1	0	1.643311	2.908256	-0.130561
43	1	0	2.427147	3.007316	1.457090
44	6	0	2.970814	1.311953	0.245749
45	6	0	4.348277	1.540962	0.333933
46	6	0	3.316604	-0.692259	-0.885130
47	6	0	5.223576	0.610175	-0.230039
48	1	0	4.721445	2.429292	0.833052
49	6	0	4.702118	-0.524074	-0.854017
50	1	0	6.296532	0.766946	-0.175627
51	1	0	5.334064	-1.280887	-1.303584

52	7	0	2.473923	0.212852	-0.349351
53	6	0	2.678141	-1.928245	-1.509320
54	8	0	3.419125	-2.748464	-2.073797
55	8	0	1.397635	-2.008027	-1.373093
56	6	0	1.515230	-2.504320	1.862195
57	1	0	2.401493	-2.274674	1.269579
58	1	0	1.829929	-2.906580	2.837742
59	1	0	0.938241	-3.265238	1.333828
60	8	0	-0.337429	-0.165132	-3.270124
61	1	0	-0.348711	0.811515	-3.151944
62	1	0	-1.280352	-0.432619	-3.160665
63	57	0	-0.202351	-0.294401	-0.509142

E(RTPSSh) = -1612.50819710

Zero-point correction= 0.517893 (Hartree/Particle)

Thermal correction to Energy= 0.549508

Thermal correction to Enthalpy= 0.550452

Thermal correction to Gibbs Free Energy= 0.458179

Sum of electronic and zero-point Energies= -1611.990304

Sum of electronic and thermal Energies= -1611.958689

Sum of electronic and thermal Enthalpies= -1611.957745

Sum of electronic and thermal Free Energies= -1612.050018

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.921754	1.575560	1.494581
2	6	0	-0.067515	2.598544	1.929352
3	6	0	-1.000871	3.044203	0.812473
4	7	0	-1.806763	1.931262	0.248723
5	6	0	-2.919963	1.582747	1.163140
6	6	0	-3.533688	0.220736	0.857708
7	7	0	-2.565475	-0.906553	0.966968
8	6	0	-2.354278	-1.266996	2.394243

9	6	0	-1.055294	-2.034016	2.635429
10	7	0	0.174280	-1.284073	2.258003
11	6	0	0.437303	-0.185054	3.220516
12	6	0	1.429761	0.847858	2.692870
13	6	0	-2.313669	2.356364	-1.072777
14	6	0	-1.187919	2.444036	-2.117048
15	8	0	-1.353004	3.145605	-3.119437
16	8	0	-0.139883	1.703788	-1.875312
17	6	0	-3.123599	-2.058672	0.217697
18	6	0	-3.080475	-1.848895	-1.309045
19	8	0	-3.793541	-2.558740	-2.024743
20	8	0	-2.244776	-0.939945	-1.721169
21	1	0	-2.840505	3.320005	-1.015079
22	1	0	-3.021756	1.605306	-1.436971
23	1	0	-4.156271	-2.272958	0.528276
24	1	0	-2.525997	-2.949522	0.442132
25	6	0	2.051744	2.257764	0.812596
26	1	0	1.634711	2.875803	0.009909
27	1	0	2.578956	2.930221	1.506208
28	6	0	3.027318	1.271206	0.209006
29	6	0	4.393345	1.546301	0.086594
30	6	0	3.303401	-0.830446	-0.756621
31	6	0	5.221985	0.587647	-0.500896
32	1	0	4.795564	2.486997	0.448481
33	6	0	4.672955	-0.624258	-0.924663
34	1	0	6.284977	0.779735	-0.610056
35	1	0	5.273593	-1.409713	-1.368111
36	1	0	-1.053865	-2.958634	2.049420
37	1	0	-1.013662	-2.328089	3.696227
38	1	0	-2.364864	-0.344697	2.980102
39	1	0	-3.192332	-1.877580	2.763000
40	1	0	0.824255	-0.595838	4.166372
41	1	0	-0.512562	0.299815	3.454663
42	1	0	1.661313	1.561395	3.498440
43	1	0	2.368511	0.361363	2.419511
44	1	0	0.450850	3.480611	2.335578

45	1	0	-0.646603	2.175814	2.752623
46	1	0	-0.419914	3.476330	-0.006063
47	1	0	-1.658109	3.841345	1.194543
48	1	0	-2.534155	1.595963	2.185935
49	1	0	-3.714116	2.344810	1.117837
50	1	0	-4.385051	0.053218	1.534796
51	1	0	-3.929465	0.212754	-0.160411
52	7	0	2.502870	0.108308	-0.214532
53	6	0	2.632681	-2.142879	-1.145028
54	8	0	3.335350	-3.033067	-1.649576
55	8	0	1.369466	-2.204195	-0.890226
56	8	0	-0.051285	-0.646145	-3.161255
57	1	0	-0.022932	0.337382	-3.190308
58	1	0	-1.012508	-0.855739	-3.068896
59	57	0	-0.180381	-0.308423	-0.381598
60	6	0	1.309359	-2.239205	2.283224
61	1	0	1.132687	-3.030176	1.553024
62	1	0	2.233545	-1.727826	2.009477
63	1	0	1.426665	-2.679829	3.285381

E(RTPSSh) = -1612.51009488

Zero-point correction= 0.517770 (Hartree/Particle)

Thermal correction to Energy= 0.549438

Thermal correction to Enthalpy= 0.550382

Thermal correction to Gibbs Free Energy= 0.457502

Sum of electronic and zero-point Energies= -1611.992325

Sum of electronic and thermal Energies= -1611.960657

Sum of electronic and thermal Enthalpies= -1611.959713

Sum of electronic and thermal Free Energies= -1612.052593

[Nd(1,4-Medo2ampa)(H_2O)]

F1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.693878	1.746332	1.323386
2	6	0	-0.328124	2.833924	1.406345
3	6	0	-1.759075	2.307593	1.510015
4	7	0	-2.192884	1.504843	0.336076
5	6	0	-3.431833	0.747596	0.660164
6	6	0	-3.171471	-0.452918	1.564818
7	7	0	-2.211306	-1.444687	1.002603
8	6	0	-1.640604	-2.253161	2.121192
9	6	0	-0.562810	-1.497516	2.897181
10	7	0	0.646711	-1.211515	2.078399
11	6	0	1.498614	-0.196901	2.755791
12	6	0	0.937646	1.221195	2.699054
13	6	0	-2.441259	2.388748	-0.826597
14	6	0	-1.164676	2.804678	-1.572790
15	8	0	-1.146007	3.873877	-2.190039
16	8	0	-0.196361	1.931805	-1.540618
17	6	0	-2.905525	-2.330278	0.030028
18	6	0	-3.061061	-1.722026	-1.377402
19	8	0	-4.016618	-2.069885	-2.077041
20	8	0	-2.105250	-0.916022	-1.740182
21	1	0	-3.013032	3.282363	-0.540274
22	1	0	-3.039016	1.823023	-1.549692
23	1	0	-3.888125	-2.642296	0.407442
24	1	0	-2.297253	-3.233408	-0.096186
25	1	0	-0.224315	3.465054	0.522858
26	1	0	-0.131627	3.474167	2.279054
27	1	0	-2.433236	3.167735	1.648291
28	1	0	-1.860574	1.685066	2.402358
29	1	0	-4.171924	1.397656	1.152509
30	1	0	-3.870871	0.417042	-0.283353
31	1	0	-4.131546	-0.946599	1.777009
32	1	0	-2.779933	-0.113186	2.525981
33	1	0	-2.433297	-2.562180	2.818375
34	1	0	-1.220121	-3.164935	1.689872

35	1	0	-0.962602	-0.549359	3.264266
36	1	0	-0.285119	-2.088144	3.784263
37	1	0	2.482332	-0.231941	2.283859
38	1	0	1.640488	-0.465018	3.815215
39	1	0	-0.011305	1.261997	3.238533
40	1	0	1.627603	1.887842	3.237791
41	6	0	1.938698	2.319259	0.738656
42	1	0	1.631681	2.925895	-0.119685
43	1	0	2.439562	2.982148	1.458844
44	6	0	2.911934	1.282715	0.221052
45	6	0	4.296575	1.482699	0.243399
46	6	0	3.171333	-0.766543	-0.864303
47	6	0	5.126351	0.519987	-0.336182
48	1	0	4.711129	2.372518	0.705685
49	6	0	4.558520	-0.623233	-0.902328
50	1	0	6.203362	0.656775	-0.333588
51	1	0	5.157209	-1.405783	-1.353445
52	7	0	2.373816	0.177895	-0.326254
53	6	0	2.475056	-2.018706	-1.389159
54	8	0	3.159858	-2.860527	-1.990298
55	8	0	1.213183	-2.089556	-1.126066
56	6	0	1.446025	-2.454346	1.951425
57	1	0	2.350631	-2.242709	1.381096
58	1	0	1.727447	-2.836648	2.944773
59	1	0	0.880469	-3.220153	1.419784
60	8	0	0.095062	-0.174863	-3.090577
61	1	0	0.007173	0.803630	-3.026668
62	1	0	-0.831395	-0.500650	-3.147946
63	60	0	-0.197369	-0.232087	-0.405835

E(RTPSSh) = -1614.41315935

Zero-point correction= 0.517809 (Hartree/Particle)

Thermal correction to Energy= 0.549616

Thermal correction to Enthalpy= 0.550560

Thermal correction to Gibbs Free Energy= 0.457225

Sum of electronic and zero-point Energies= -1613.895350

Sum of electronic and thermal Energies= -1613.863543

Sum of electronic and thermal Enthalpies= -1613.862599

Sum of electronic and thermal Free Energies= -1613.955935

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.848233	1.601352	1.517596
2	6	0	-0.165627	2.605206	1.943424
3	6	0	-1.100504	3.033001	0.821532
4	7	0	-1.857047	1.900423	0.225034
5	6	0	-2.989939	1.501365	1.092608
6	6	0	-3.532391	0.120369	0.733991
7	7	0	-2.521148	-0.966531	0.868712
8	6	0	-2.360745	-1.340770	2.300181
9	6	0	-1.048716	-2.067984	2.583576
10	7	0	0.169022	-1.281081	2.240749
11	6	0	0.369005	-0.178244	3.215955
12	6	0	1.351577	0.879748	2.721414
13	6	0	-2.326600	2.324830	-1.110789
14	6	0	-1.160925	2.428207	-2.106789
15	8	0	-1.309046	3.080724	-3.143565
16	8	0	-0.091065	1.755154	-1.778996
17	6	0	-2.989452	-2.131021	0.075639
18	6	0	-2.844261	-1.909753	-1.443430
19	8	0	-3.550028	-2.568011	-2.211416
20	8	0	-1.926900	-1.052483	-1.794955
21	1	0	-2.864681	3.282791	-1.066750
22	1	0	-3.018035	1.573752	-1.505282
23	1	0	-4.032841	-2.379406	0.313489
24	1	0	-2.377931	-3.002633	0.335472
25	6	0	1.976749	2.285039	0.832664
26	1	0	1.555921	2.907832	0.035940
27	1	0	2.514279	2.948763	1.526241

28	6	0	2.938460	1.289227	0.216505
29	6	0	4.305970	1.542490	0.069731
30	6	0	3.172587	-0.833994	-0.728534
31	6	0	5.109963	0.565158	-0.522812
32	1	0	4.729671	2.478994	0.417447
33	6	0	4.540765	-0.646099	-0.923610
34	1	0	6.173548	0.741640	-0.650801
35	1	0	5.127164	-1.443442	-1.365008
36	1	0	-1.001509	-2.992892	2.000598
37	1	0	-1.030617	-2.358348	3.645894
38	1	0	-2.424487	-0.427463	2.896239
39	1	0	-3.194105	-1.982362	2.622941
40	1	0	0.732652	-0.582239	4.173650
41	1	0	-0.600276	0.282381	3.417628
42	1	0	1.549919	1.593538	3.535088
43	1	0	2.306684	0.416613	2.464490
44	1	0	0.330006	3.497339	2.355224
45	1	0	-0.742487	2.167578	2.760766
46	1	0	-0.523883	3.499887	0.019823
47	1	0	-1.793160	3.797123	1.207073
48	1	0	-2.645065	1.512921	2.130283
49	1	0	-3.811419	2.231764	1.026741
50	1	0	-4.407954	-0.098710	1.363247
51	1	0	-3.878489	0.115688	-0.302960
52	7	0	2.397844	0.127445	-0.189994
53	6	0	2.469142	-2.145468	-1.062622
54	8	0	3.132757	-3.046930	-1.597290
55	8	0	1.224639	-2.195859	-0.721005
56	8	0	0.458588	-0.508645	-2.952952
57	1	0	0.347614	0.470735	-3.006325
58	1	0	-0.450975	-0.862003	-3.075883
59	6	0	1.328404	-2.204435	2.315831
60	1	0	1.191594	-3.011873	1.597030
61	1	0	2.245965	-1.673717	2.057740
62	1	0	1.426252	-2.619230	3.330831
63	60	0	-0.174400	-0.236152	-0.324015

E(RTPSSh) = -1614.41563507

Zero-point correction= 0.518089 (Hartree/Particle)

Thermal correction to Energy= 0.549659

Thermal correction to Enthalpy= 0.550603

Thermal correction to Gibbs Free Energy= 0.458305

Sum of electronic and zero-point Energies= -1613.897546

Sum of electronic and thermal Energies= -1613.865976

Sum of electronic and thermal Enthalpies= -1613.865032

Sum of electronic and thermal Free Energies= -1613.957330

[Eu(1,4-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.594857	1.674579	1.423847
2	6	0	-0.465198	2.716129	1.583047
3	6	0	-1.873127	2.125822	1.657440
4	7	0	-2.275465	1.369860	0.441541
5	6	0	-3.456997	0.514579	0.732775
6	6	0	-3.101839	-0.728878	1.540988
7	7	0	-2.097886	-1.617014	0.888726
8	6	0	-1.483687	-2.491570	1.926478
9	6	0	-0.447956	-1.747109	2.761889
10	7	0	0.724469	-1.310009	1.958369
11	6	0	1.512513	-0.306239	2.722226
12	6	0	0.866320	1.074567	2.761463
13	6	0	-2.600373	2.305702	-0.659904
14	6	0	-1.366781	2.832024	-1.403569
15	8	0	-1.442183	3.891045	-2.032445
16	8	0	-0.320384	2.056519	-1.348333
17	6	0	-2.755087	-2.444942	-0.156070

18	6	0	-2.945625	-1.700254	-1.490570
19	8	0	-3.897662	-2.008872	-2.216748
20	8	0	-2.028790	-0.824442	-1.767090
21	1	0	-3.211331	3.148548	-0.307938
22	1	0	-3.186068	1.755559	-1.403886
23	1	0	-3.718935	-2.838410	0.193344
24	1	0	-2.103405	-3.300366	-0.367847
25	1	0	-0.390313	3.407622	0.743491
26	1	0	-0.287408	3.302584	2.496714
27	1	0	-2.582186	2.948304	1.841854
28	1	0	-1.948429	1.453209	2.515701
29	1	0	-4.223884	1.079589	1.285046
30	1	0	-3.897456	0.225306	-0.223271
31	1	0	-4.025264	-1.295039	1.736006
32	1	0	-2.708152	-0.435155	2.516172
33	1	0	-2.255587	-2.904634	2.592821
34	1	0	-1.015594	-3.336218	1.415095
35	1	0	-0.900265	-0.865344	3.222042
36	1	0	-0.116497	-2.397841	3.586277
37	1	0	2.501895	-0.250175	2.264851
38	1	0	1.659429	-0.644828	3.760475
39	1	0	-0.086427	1.016493	3.292671
40	1	0	1.510188	1.744887	3.350671
41	6	0	1.816651	2.325091	0.871718
42	1	0	1.485541	2.961583	0.044714
43	1	0	2.294834	2.966468	1.625678
44	6	0	2.821122	1.344652	0.306552
45	6	0	4.202273	1.564731	0.358177
46	6	0	3.129348	-0.648108	-0.867915
47	6	0	5.055672	0.640190	-0.248564
48	1	0	4.596150	2.438658	0.866411
49	6	0	4.514757	-0.487091	-0.871025
50	1	0	6.130290	0.791905	-0.222204
51	1	0	5.132626	-1.243830	-1.339943
52	7	0	2.309014	0.261640	-0.304362
53	6	0	2.455949	-1.882924	-1.461569

54	8	0	3.168472	-2.718639	-2.038061
55	8	0	1.178221	-1.941835	-1.285153
56	63	0	-0.210992	-0.166018	-0.433310
57	6	0	1.597029	-2.488361	1.734258
58	1	0	2.504195	-2.176525	1.215862
59	1	0	1.878390	-2.948039	2.694333
60	1	0	1.086864	-3.227285	1.116325
61	8	0	0.545564	0.285052	-2.930734
62	1	0	1.484308	0.160383	-3.152124
63	1	0	0.424419	1.249635	-2.756106

E(RTPSSh) = -1616.22863759

Zero-point correction= 0.517911 (Hartree/Particle)

Thermal correction to Energy= 0.549627

Thermal correction to Enthalpy= 0.550571

Thermal correction to Gibbs Free Energy= 0.458331

Sum of electronic and zero-point Energies= -1615.710726

Sum of electronic and thermal Energies= -1615.679011

Sum of electronic and thermal Enthalpies= -1615.678067

Sum of electronic and thermal Free Energies= -1615.770307

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.822433	1.751417	1.322893
2	6	0	-0.196843	2.771776	1.690000
3	6	0	-1.158131	3.090125	0.554663
4	7	0	-1.881591	1.887279	0.062999
5	6	0	-3.023276	1.571093	0.953321
6	6	0	-3.528056	0.146380	0.757857
7	7	0	-2.477175	-0.888165	0.981691
8	6	0	-2.288595	-1.124201	2.436306
9	6	0	-0.964707	-1.814544	2.750406
10	7	0	0.232622	-1.050160	2.303239

11	6	0	0.449193	0.125266	3.188088
12	6	0	1.383641	1.160117	2.571185
13	6	0	-2.317911	2.146979	-1.326765
14	6	0	-1.099365	2.188652	-2.269033
15	8	0	-1.207046	2.739501	-3.370038
16	8	0	-0.034182	1.598458	-1.811751
17	6	0	-2.919485	-2.132719	0.307508
18	6	0	-2.820389	-2.014629	-1.222347
19	8	0	-3.464223	-2.788149	-1.933954
20	8	0	-2.001113	-1.089681	-1.643244
21	1	0	-2.886890	3.084187	-1.408344
22	1	0	-2.962629	1.326832	-1.657597
23	1	0	-3.946302	-2.400149	0.593458
24	1	0	-2.268835	-2.958253	0.616133
25	6	0	1.914464	2.384611	0.537036
26	1	0	1.459446	2.891021	-0.319828
27	1	0	2.447993	3.137204	1.136117
28	6	0	2.886648	1.341525	0.029664
29	6	0	4.252801	1.590990	-0.136726
30	6	0	3.155972	-0.877366	-0.633072
31	6	0	5.077365	0.556089	-0.584571
32	1	0	4.660038	2.570457	0.091504
33	6	0	4.526649	-0.705122	-0.822070
34	1	0	6.140450	0.727349	-0.722227
35	1	0	5.127618	-1.550452	-1.135941
36	1	0	-0.923206	-2.789065	2.254677
37	1	0	-0.913681	-2.005716	3.833825
38	1	0	-2.344854	-0.158921	2.945228
39	1	0	-3.110083	-1.736993	2.836760
40	1	0	0.864538	-0.200699	4.154300
41	1	0	-0.519331	0.581154	3.402140
42	1	0	1.585592	1.950367	3.309573
43	1	0	2.342770	0.697997	2.328246
44	1	0	0.293468	3.700049	2.020285
45	1	0	-0.752196	2.389917	2.549721
46	1	0	-0.609037	3.517721	-0.286320

47	1	0	-1.872345	3.855691	0.893752
48	1	0	-2.695021	1.718221	1.986029
49	1	0	-3.857288	2.269896	0.785580
50	1	0	-4.381873	-0.031587	1.428209
51	1	0	-3.893184	0.024265	-0.264608
52	7	0	2.357836	0.134427	-0.240240
53	6	0	2.477799	-2.225510	-0.817422
54	8	0	3.174452	-3.207277	-1.106455
55	8	0	1.191081	-2.216363	-0.642733
56	63	0	-0.194830	-0.204678	-0.311440
57	8	0	0.294537	-1.068463	-2.870067
58	1	0	-0.684948	-1.187573	-2.893108
59	1	0	0.617786	-1.905644	-2.475930
60	6	0	1.401869	-1.956255	2.419119
61	1	0	1.258928	-2.812725	1.760485
62	1	0	2.310881	-1.435021	2.114397
63	1	0	1.521720	-2.302176	3.457165

E(RTPSSh) = -1616.22975927

Zero-point correction= 0.518268 (Hartree/Particle)

Thermal correction to Energy= 0.549764

Thermal correction to Enthalpy= 0.550708

Thermal correction to Gibbs Free Energy= 0.458927

Sum of electronic and zero-point Energies= -1615.711492

Sum of electronic and thermal Energies= -1615.679995

Sum of electronic and thermal Enthalpies= -1615.679051

Sum of electronic and thermal Free Energies= -1615.770832

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.665844	0.199620	2.166479
2	7	0	-1.900554	1.430992	1.036055
3	6	0	-3.226164	0.769945	1.161746

4	6	0	-3.149906	-0.743710	1.337659
5	7	0	-2.460204	-1.446783	0.219911
6	6	0	-2.147229	-2.839416	0.651471
7	6	0	-0.904569	-2.899202	1.534899
8	7	0	0.313913	-2.439915	0.819551
9	6	0	1.433021	-2.208479	1.767323
10	6	0	1.189445	-1.074075	2.765727
11	6	0	-2.045684	2.691212	0.268686
12	6	0	-0.679194	3.218998	-0.183229
13	8	0	-0.528675	4.424258	-0.404425
14	8	0	0.231643	2.298449	-0.355441
15	6	0	-3.331313	-1.465639	-0.983152
16	6	0	-3.229387	-0.203205	-1.855379
17	8	0	-4.200986	0.143301	-2.532618
18	8	0	-2.063324	0.376723	-1.849015
19	1	0	-2.576319	3.464244	0.841479
20	1	0	-2.619892	2.475719	-0.637783
21	1	0	-4.380870	-1.644432	-0.714479
22	1	0	-3.007658	-2.296407	-1.619963
23	1	0	-3.792033	1.188426	2.007581
24	1	0	-3.798148	0.999443	0.259035
25	1	0	-4.175287	-1.132835	1.438915
26	1	0	-2.630230	-0.988635	2.265300
27	1	0	-2.997625	-3.278671	1.193686
28	1	0	-1.995012	-3.442012	-0.246555
29	1	0	-1.045948	-2.271873	2.417253
30	1	0	-0.768427	-3.930195	1.897234
31	1	0	2.317119	-2.000298	1.162610
32	1	0	1.640121	-3.123270	2.347226
33	1	0	0.484732	-1.402965	3.533504
34	1	0	2.134445	-0.881164	3.288558
35	6	0	1.748939	1.217496	2.112458
36	1	0	1.303231	2.171994	1.819380
37	1	0	2.212185	1.345076	3.101780
38	6	0	2.796997	0.861478	1.082036
39	6	0	4.152811	1.170829	1.231409

40	6	0	5.036761	0.835287	0.202144
41	6	0	3.192978	-0.118560	-0.996624
42	6	0	4.554605	0.176622	-0.931377
43	1	0	5.202762	-0.124066	-1.746339
44	1	0	4.505900	1.658901	2.133976
45	1	0	6.092771	1.070043	0.294480
46	6	0	-0.459605	0.698081	3.008162
47	6	0	-1.298916	1.788261	2.353111
48	1	0	-1.090484	-0.160032	3.245350
49	1	0	-0.082790	1.086701	3.967427
50	1	0	-2.087383	2.081345	3.062557
51	1	0	-0.680707	2.676539	2.199324
52	6	0	2.571687	-0.908348	-2.140141
53	8	0	3.282041	-1.212441	-3.110356
54	8	0	1.329672	-1.214427	-1.959959
55	7	0	2.341676	0.238601	-0.017539
56	63	0	-0.174026	-0.080312	-0.482284
57	6	0	0.743967	-3.505050	-0.121139
58	1	0	1.665938	-3.197715	-0.611963
59	1	0	0.903484	-4.452319	0.416267
60	1	0	-0.011462	-3.656089	-0.894169
61	8	0	0.224963	1.291416	-2.799049
62	1	0	-0.752654	1.241936	-2.898082
63	1	0	0.370988	2.071248	-2.218733

E(RTPSSh) = -1616.22092380

Zero-point correction= 0.518658 (Hartree/Particle)

Thermal correction to Energy= 0.550160

Thermal correction to Enthalpy= 0.551105

Thermal correction to Gibbs Free Energy= 0.459177

Sum of electronic and zero-point Energies= -1615.702266

Sum of electronic and thermal Energies= -1615.670763

Sum of electronic and thermal Enthalpies= -1615.669819

Sum of electronic and thermal Free Energies= -1615.761747

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.803717	-1.964389	1.212943
2	7	0	-1.833286	-0.596767	1.752985
3	7	0	-2.486851	-0.715690	-1.217524
4	6	0	-2.316843	-2.000446	-1.966560
5	6	0	-1.047230	-2.765237	-1.585053
6	7	0	0.187431	-1.947178	-1.696975
7	6	0	1.366220	-2.680670	-1.164523
8	6	0	1.248093	-3.075403	0.309024
9	6	0	-2.305304	0.656050	2.385380
10	6	0	-1.149902	1.650106	2.597039
11	8	0	-1.302635	2.597059	3.369606
12	8	0	-0.075215	1.422289	1.883554
13	6	0	-2.939637	0.367462	-2.132228
14	6	0	-2.784850	1.760211	-1.491112
15	8	0	-3.453874	2.697853	-1.935020
16	8	0	-1.906585	1.833093	-0.534406
17	1	0	-2.808673	0.460841	3.342355
18	1	0	-3.020441	1.146362	1.718860
19	1	0	-3.979471	0.219957	-2.452760
20	1	0	-2.310217	0.350439	-3.028892
21	1	0	-3.176638	-2.659279	-1.792695
22	1	0	-2.311298	-1.776196	-3.035841
23	1	0	-1.134783	-3.098403	-0.548901
24	1	0	-0.973361	-3.668032	-2.212030
25	1	0	2.234969	-2.036041	-1.320475
26	1	0	1.536665	-3.603006	-1.743324
27	1	0	0.545753	-3.905272	0.414283
28	1	0	2.223055	-3.460861	0.632900
29	6	0	1.970448	-1.417228	1.960164
30	1	0	1.589560	-0.713868	2.708683
31	1	0	2.499265	-2.220481	2.492535

32	6	0	2.920660	-0.667232	1.056115
33	6	0	4.310454	-0.796411	1.125844
34	6	0	5.103054	-0.026568	0.269089
35	6	0	3.098057	0.927920	-0.633857
36	6	0	4.491070	0.850855	-0.627110
37	1	0	5.059107	1.467117	-1.314046
38	1	0	4.758869	-1.488741	1.830404
39	1	0	6.184329	-0.116531	0.300169
40	6	0	-0.205536	-2.471057	2.189017
41	6	0	-1.079488	-1.370421	2.778300
42	1	0	-0.829792	-3.201480	1.669636
43	1	0	0.284304	-3.010267	3.013143
44	1	0	-1.775040	-1.822879	3.501099
45	1	0	-0.462161	-0.657072	3.329871
46	6	0	-3.492199	-0.819433	-0.114970
47	6	0	-2.953369	-1.398227	1.190721
48	1	0	-3.872991	0.187978	0.069287
49	1	0	-4.347541	-1.426699	-0.443055
50	1	0	-3.780548	-1.466471	1.913120
51	1	0	-2.593212	-2.416612	1.026242
52	7	0	2.338205	0.178995	0.187054
53	6	0	2.342777	1.865412	-1.559808
54	8	0	2.971662	2.523771	-2.394237
55	8	0	1.054267	1.895637	-1.365057
56	63	0	-0.213817	0.257015	-0.154758
57	6	0	0.464486	-1.629772	-3.120462
58	1	0	1.405030	-1.078101	-3.185809
59	1	0	0.545105	-2.547321	-3.721407
60	1	0	-0.328879	-1.003951	-3.533249
61	8	0	0.899983	3.832998	0.774524
62	1	0	0.882440	3.387263	-0.096424
63	1	0	0.615971	3.099776	1.364938

E(RTPSSh) = -1616.22292469

Zero-point correction= 0.517614 (Hartree/Particle)

Thermal correction to Energy= 0.549682

Thermal correction to Enthalpy= 0.550626

Thermal correction to Gibbs Free Energy= 0.456830

Sum of electronic and zero-point Energies= -1615.705311

Sum of electronic and thermal Energies= -1615.673243

Sum of electronic and thermal Enthalpies= -1615.672299

Sum of electronic and thermal Free Energies= -1615.766095

F5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.491516	-0.346722	2.155832
2	7	0	-1.932901	1.280646	1.260173
3	6	0	-3.273505	0.650875	1.189114
4	6	0	-3.234810	-0.875281	1.257443
5	7	0	-2.319816	-1.503356	0.257643
6	6	0	1.372548	-2.555635	1.238205
7	6	0	0.828292	-1.778924	2.434422
8	6	0	-1.998480	2.668204	0.747596
9	6	0	-0.605359	3.170663	0.328184
10	8	0	-0.510227	4.320074	-0.134899
11	8	0	0.354513	2.308359	0.417744
12	6	0	-3.049711	-1.702558	-1.023588
13	6	0	-3.204785	-0.416887	-1.846388
14	8	0	-4.201915	-0.258036	-2.554901
15	8	0	-2.197218	0.402022	-1.753773
16	1	0	-2.448781	3.362998	1.471624
17	1	0	-2.628291	2.675711	-0.147565
18	1	0	-4.034416	-2.154568	-0.844219
19	1	0	-2.474552	-2.397239	-1.645216
20	1	0	-3.923581	1.014240	2.000471
21	1	0	-3.726548	0.964820	0.246745
22	1	0	-4.258823	-1.253229	1.122233
23	1	0	-2.921649	-1.195863	2.251531
24	1	0	2.367492	-2.186405	0.984322

25	1	0	1.488864	-3.607307	1.546514
26	1	0	-0.068649	-2.267304	2.814842
27	1	0	1.572313	-1.840418	3.241781
28	6	0	1.679990	0.514507	2.416710
29	1	0	1.337387	1.553601	2.413585
30	1	0	2.098700	0.293228	3.409053
31	6	0	2.749043	0.396524	1.355268
32	6	0	4.112466	0.537029	1.635387
33	6	0	5.024554	0.501934	0.577095
34	6	0	3.184750	0.169768	-0.923635
35	6	0	4.557703	0.319336	-0.726447
36	1	0	5.222719	0.282320	-1.581316
37	1	0	4.449179	0.671495	2.658139
38	1	0	6.087199	0.610633	0.771281
39	6	0	-0.608265	0.071271	3.076261
40	6	0	-1.361433	1.324902	2.636053
41	1	0	-1.296382	-0.768458	3.159504
42	1	0	-0.213500	0.250253	4.088347
43	1	0	-2.160372	1.513813	3.369405
44	1	0	-0.685203	2.181064	2.674375
45	6	0	-1.862503	-2.822878	0.771139
46	6	0	-0.643538	-3.366521	0.033173
47	7	0	0.556281	-2.478202	-0.005448
48	1	0	-0.913369	-3.564229	-1.008471
49	1	0	-0.375865	-4.338378	0.476444
50	1	0	-1.650621	-2.712623	1.834435
51	1	0	-2.666251	-3.571417	0.690851
52	7	0	2.311574	0.209067	0.099004
53	6	0	2.572341	-0.059373	-2.299251
54	8	0	3.323617	-0.089082	-3.285244
55	8	0	1.289496	-0.216809	-2.295996
56	63	0	-0.190081	0.149470	-0.461636
57	6	0	1.410003	-3.005452	-1.105004
58	1	0	0.893678	-2.885580	-2.058578
59	1	0	2.346287	-2.448792	-1.141503
60	1	0	1.636970	-4.070198	-0.943066

61	8	0	-0.420654	2.156024	-2.314965
62	1	0	-1.346508	1.857613	-2.466264
63	1	0	-0.475624	3.054144	-1.930824

E(RTPSSh) = -1616.21530660

Zero-point correction= 0.519023 (Hartree/Particle)

Thermal correction to Energy= 0.550383

Thermal correction to Enthalpy= 0.551328

Thermal correction to Gibbs Free Energy= 0.460045

Sum of electronic and zero-point Energies= -1615.696284

Sum of electronic and thermal Energies= -1615.664923

Sum of electronic and thermal Enthalpies= -1615.663979

Sum of electronic and thermal Free Energies= -1615.755262

F6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.151359	-2.132606	0.441316
2	7	0	0.765670	-1.860018	-1.841874
3	6	0	2.254616	-1.904993	-1.898122
4	6	0	2.930745	-1.722835	-0.541943
5	7	0	2.667863	-0.395451	0.079199
6	6	0	3.086290	-0.398378	1.507682
7	6	0	2.178343	-1.238068	2.402311
8	7	0	0.738561	-0.859463	2.336135
9	6	0	3.416746	0.664403	-0.640830
10	6	0	2.712317	1.159911	-1.911789
11	8	0	3.387541	1.615285	-2.840889
12	8	0	1.412713	1.108797	-1.875720
13	6	0	0.461881	0.286752	3.240739
14	6	0	0.934283	1.637211	2.689582
15	8	0	1.298304	2.525195	3.462803
16	8	0	0.856525	1.748315	1.392665
17	1	0	4.440047	0.343128	-0.877749

18	1	0	3.477705	1.535551	0.019875
19	1	0	-0.625323	0.362308	3.363300
20	1	0	0.900679	0.117426	4.233360
21	1	0	2.586946	-2.863450	-2.323949
22	1	0	2.583914	-1.124778	-2.587356
23	1	0	4.015238	-1.864260	-0.672794
24	1	0	2.594603	-2.502245	0.144755
25	1	0	4.113270	-0.782659	1.610093
26	1	0	3.095580	0.639791	1.843129
27	1	0	2.258733	-2.290969	2.121900
28	1	0	2.548736	-1.164058	3.435735
29	6	0	-2.470914	-2.304472	-0.218179
30	1	0	-2.305490	-2.571189	-1.265921
31	1	0	-3.032150	-3.130752	0.240375
32	6	0	-3.275024	-1.026670	-0.194349
33	6	0	-4.665313	-1.003957	-0.051227
34	6	0	-5.328312	0.223333	-0.129304
35	6	0	-3.203759	1.279983	-0.480791
36	6	0	-4.589108	1.385772	-0.355066
37	1	0	-5.053596	2.361817	-0.432578
38	1	0	-5.211365	-1.926340	0.116719
39	1	0	-6.407155	0.268274	-0.016844
40	6	0	-0.231741	-3.232043	0.052913
41	6	0	0.190377	-3.173876	-1.415390
42	1	0	0.656465	-3.150865	0.679566
43	1	0	-0.680829	-4.216986	0.254845
44	1	0	0.914510	-3.980705	-1.589511
45	1	0	-0.664139	-3.390701	-2.061425
46	6	0	-1.393981	-2.104795	1.913539
47	6	0	-0.120491	-2.010614	2.745938
48	1	0	-1.945497	-3.005339	2.225559
49	1	0	-2.040123	-1.242581	2.112644
50	1	0	-0.404261	-1.929111	3.802920
51	1	0	0.455261	-2.934235	2.660355
52	7	0	-2.565229	0.097645	-0.391996
53	6	0	-2.316663	2.484068	-0.751151

54	8	0	-1.058173	2.207903	-0.868987
55	8	0	-2.842136	3.601920	-0.851506
56	63	0	0.069806	0.224107	-0.196957
57	6	0	0.262603	-1.538665	-3.205867
58	1	0	0.552002	-2.311360	-3.932300
59	1	0	-0.828027	-1.465407	-3.181422
60	1	0	0.672022	-0.574593	-3.511722
61	8	0	1.701751	3.852454	-0.220969
62	1	0	1.435714	3.227699	0.494253
63	1	0	1.260612	3.445750	-0.988334

E(RTPSSh) = -1616.21926210

Zero-point correction= 0.517380 (Hartree/Particle)

Thermal correction to Energy= 0.549956

Thermal correction to Enthalpy= 0.550900

Thermal correction to Gibbs Free Energy= 0.453962

Sum of electronic and zero-point Energies= -1615.701882

Sum of electronic and thermal Energies= -1615.669306

Sum of electronic and thermal Enthalpies= -1615.668362

Sum of electronic and thermal Free Energies= -1615.765300

F7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.646871	-2.579960	0.338167
2	7	0	1.600488	-1.937784	-1.534314
3	7	0	2.606963	-0.212949	0.699648
4	6	0	2.463115	-0.786274	2.060879
5	6	0	1.290932	-0.197545	2.853160
6	7	0	-0.067221	-0.253189	2.206168
7	6	0	-0.838385	-1.472975	2.580736
8	6	0	-0.438310	-2.718659	1.804979
9	6	0	3.181899	1.152354	0.707270
10	6	0	2.958422	1.837144	-0.656723

11	8	0	3.650319	2.817957	-0.950437
12	8	0	2.020306	1.317548	-1.394268
13	6	0	-0.824495	0.933863	2.689758
14	6	0	-0.286564	2.229794	2.071942
15	8	0	-0.497720	3.308434	2.632834
16	8	0	0.336744	2.067803	0.940869
17	1	0	4.254311	1.134090	0.947084
18	1	0	2.670751	1.755380	1.460771
19	1	0	-1.869445	0.830378	2.375749
20	1	0	-0.811782	1.002850	3.785367
21	1	0	-1.895055	-1.256928	2.398193
22	1	0	-0.733460	-1.675727	3.656602
23	1	0	0.617047	-2.939285	1.975265
24	1	0	-1.008946	-3.573196	2.200347
25	6	0	-2.081606	-2.749909	-0.014289
26	1	0	-2.116707	-3.162535	-1.029292
27	1	0	-2.552380	-3.493517	0.643835
28	6	0	-2.920752	-1.494745	-0.070916
29	6	0	-4.292680	-1.531914	0.205988
30	6	0	-5.069879	-0.405751	-0.068959
31	6	0	-3.086915	0.686037	-0.858821
32	6	0	-4.462508	0.716615	-0.634274
33	1	0	-5.019989	1.605945	-0.903313
34	1	0	-4.739189	-2.433100	0.613222
35	1	0	-6.135517	-0.412775	0.137580
36	6	0	0.129783	-3.630060	-0.387727
37	6	0	0.703390	-3.113991	-1.701920
38	1	0	0.924166	-3.992429	0.266601
39	1	0	-0.499008	-4.504646	-0.599161
40	1	0	1.239149	-3.936923	-2.201054
41	1	0	-0.109125	-2.803115	-2.368718
42	6	0	3.493892	-1.063507	-0.147083
43	6	0	2.789624	-2.289106	-0.712693
44	1	0	3.862083	-0.438572	-0.962983
45	1	0	4.370879	-1.388200	0.432277
46	1	0	3.506860	-2.874987	-1.307221

47	1	0	2.468366	-2.928106	0.110246
48	1	0	1.503473	0.856059	3.050993
49	1	0	1.249963	-0.697751	3.830659
50	1	0	3.378038	-0.624449	2.651389
51	1	0	2.348434	-1.866333	1.951719
52	7	0	-2.328071	-0.389601	-0.557130
53	6	0	-2.364221	1.851958	-1.508044
54	8	0	-3.019505	2.839728	-1.864018
55	8	0	-1.083842	1.693896	-1.646980
56	63	0	0.245438	0.117787	-0.428398
57	6	0	2.038378	-1.498690	-2.882959
58	1	0	2.588251	-2.300308	-3.397712
59	1	0	1.158174	-1.235477	-3.476984
60	1	0	2.670419	-0.614804	-2.793173
61	8	0	-0.029251	4.231606	-0.843822
62	1	0	0.218473	3.650516	-0.090364
63	1	0	-0.472993	3.568130	-1.411841

E(RTPSSh) = -1616.21637960

Zero-point correction= 0.518482 (Hartree/Particle)

Thermal correction to Energy= 0.550189

Thermal correction to Enthalpy= 0.551133

Thermal correction to Gibbs Free Energy= 0.458993

Sum of electronic and zero-point Energies= -1615.697898

Sum of electronic and thermal Energies= -1615.666190

Sum of electronic and thermal Enthalpies= -1615.665246

Sum of electronic and thermal Free Energies= -1615.757387

F8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.804775	1.961721	1.102651
2	7	0	1.690438	0.459690	1.806065
3	7	0	2.711357	0.209837	-1.071989

4	6	0	2.854919	1.330739	-2.039385
5	6	0	2.065777	2.571955	-1.647895
6	7	0	0.615291	2.296489	-1.465468
7	6	0	-0.023228	3.448355	-0.766528
8	6	0	-1.182861	3.023474	0.127219
9	6	0	1.920667	-0.829728	2.498284
10	6	0	0.621327	-1.646457	2.588662
11	8	0	0.560846	-2.600411	3.366762
12	8	0	-0.338351	-1.265730	1.784352
13	6	0	3.100228	-1.057478	-1.745351
14	6	0	2.602202	-2.291202	-0.974265
15	8	0	3.182095	-3.371081	-1.131434
16	8	0	1.553500	-2.088893	-0.235957
17	1	0	2.339137	-0.677951	3.502986
18	1	0	2.628225	-1.430474	1.922553
19	1	0	4.185916	-1.120860	-1.897238
20	1	0	2.625497	-1.080574	-2.732809
21	1	0	3.912496	1.607804	-2.161897
22	1	0	2.507016	0.967462	-3.010143
23	1	0	2.450513	2.979610	-0.710905
24	1	0	2.217520	3.343730	-2.418402
25	6	0	-2.026659	1.525247	1.828459
26	1	0	-1.717441	0.834836	2.619472
27	1	0	-2.527509	2.382243	2.301706
28	6	0	-2.981550	0.794855	0.911329
29	6	0	-4.372194	0.876178	1.033829
30	6	0	-5.169825	0.142754	0.151685
31	6	0	-3.170467	-0.683682	-0.878869
32	6	0	-4.563494	-0.645647	-0.828669
33	1	0	-5.137122	-1.226136	-1.541727
34	1	0	-4.816856	1.504362	1.798575
35	1	0	-6.251644	0.193231	0.226120
36	6	0	0.200015	2.472623	2.072766
37	6	0	0.972618	1.354022	2.758956
38	1	0	0.895501	3.117778	1.534849
39	1	0	-0.281647	3.099531	2.837719

40	1	0	1.682738	1.795293	3.473896
41	1	0	0.286816	0.729019	3.334988
42	6	0	3.580457	0.368833	0.137936
43	6	0	2.954901	1.083169	1.340328
44	1	0	3.883161	-0.634992	0.447814
45	1	0	4.502443	0.901482	-0.135145
46	1	0	3.702214	1.093713	2.149097
47	1	0	2.739996	2.126417	1.100669
48	1	0	-1.568999	3.910188	0.653182
49	1	0	-1.999202	2.628136	-0.484126
50	1	0	0.742089	3.962361	-0.181171
51	1	0	-0.393988	4.183095	-1.494469
52	7	0	-2.406506	0.024532	-0.027243
53	6	0	-2.414414	-1.540218	-1.879147
54	8	0	-3.037084	-2.100193	-2.787430
55	8	0	-1.132040	-1.620649	-1.659543
56	63	0	0.162726	-0.192438	-0.253214
57	6	0	-0.041163	2.122969	-2.786120
58	1	0	-1.118097	1.999477	-2.644082
59	1	0	0.132442	2.998283	-3.428931
60	1	0	0.339371	1.234093	-3.294716
61	8	0	-1.532500	-3.517440	0.593756
62	1	0	-1.273905	-3.161545	-0.278269
63	1	0	-1.194311	-2.811244	1.191397

E(RTPSSh) = -1616.22431193 Zero-point correction= 0.518046 (Hartree/Particle)

Thermal correction to Energy= 0.549988

Thermal correction to Enthalpy= 0.550932

Thermal correction to Gibbs Free Energy= 0.457623

Sum of electronic and zero-point Energies= -1615.706266

Sum of electronic and thermal Energies= -1615.674324

Sum of electronic and thermal Enthalpies= -1615.673380

Sum of electronic and thermal Free Energies= -1615.766689

F9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.633029	0.354828	2.108828
2	7	0	-1.856559	1.601184	0.866413
3	6	0	-3.229665	1.038729	0.947275
4	6	0	-3.272734	-0.443925	1.296525
5	7	0	-2.534162	-1.320880	0.342474
6	6	0	0.184180	-2.093635	2.439926
7	6	0	1.100981	-0.913501	2.742877
8	6	0	-1.885207	2.821061	0.023680
9	6	0	-0.467946	3.243924	-0.377719
10	8	0	-0.221714	4.430317	-0.614619
11	8	0	0.379889	2.257145	-0.490743
12	6	0	-3.289602	-1.473413	-0.929498
13	6	0	-3.153907	-0.302977	-1.915229
14	8	0	-4.090458	-0.043479	-2.675520
15	8	0	-1.997829	0.295983	-1.903105
16	1	0	-2.400756	3.653625	0.521825
17	1	0	-2.423557	2.583246	-0.899648
18	1	0	-4.352734	-1.664740	-0.729245
19	1	0	-2.885708	-2.352003	-1.446455
20	1	0	-3.828701	1.581902	1.694305
21	1	0	-3.710398	1.202219	-0.020036
22	1	0	-4.327669	-0.754421	1.357273
23	1	0	-2.841663	-0.599898	2.288057
24	6	0	1.772802	1.309125	2.057966
25	1	0	1.386692	2.285155	1.752146
26	1	0	2.232519	1.420938	3.051054
27	6	0	2.810097	0.868588	1.045044
28	6	0	4.164626	1.204595	1.140736
29	6	0	5.037476	0.768746	0.139814
30	6	0	3.188643	-0.319336	-0.928633
31	6	0	4.548549	-0.011893	-0.910802

32	1	0	5.189231	-0.391289	-1.698386
33	1	0	4.525824	1.789191	1.980645
34	1	0	6.091820	1.022901	0.190674
35	6	0	-0.482716	0.919726	2.916627
36	6	0	-1.296077	1.992063	2.194243
37	1	0	-1.128030	0.090136	3.208199
38	1	0	-0.093164	1.355903	3.849816
39	1	0	-2.103382	2.319031	2.865978
40	1	0	-0.660132	2.866746	2.032672
41	6	0	-2.365489	-2.671990	0.963471
42	6	0	-1.010284	-3.296171	0.653465
43	7	0	0.145304	-2.418703	0.991541
44	1	0	-0.931251	-3.514050	-0.417669
45	1	0	-0.937463	-4.256637	1.188454
46	1	0	-2.503699	-2.580199	2.042682
47	1	0	-3.152058	-3.355152	0.618253
48	1	0	1.174400	-0.783916	3.832871
49	1	0	2.109189	-1.117669	2.376352
50	1	0	0.518822	-2.966127	3.022164
51	1	0	-0.827872	-1.863079	2.776033
52	7	0	2.348965	0.130555	0.022314
53	6	0	2.553924	-1.209690	-1.989137
54	8	0	3.271990	-1.654158	-2.897594
55	8	0	1.294311	-1.436169	-1.813608
56	63	0	-0.154483	-0.097434	-0.459579
57	6	0	1.374520	-3.168480	0.634134
58	1	0	1.338380	-3.428689	-0.423085
59	1	0	2.256726	-2.549951	0.804318
60	1	0	1.454988	-4.083676	1.240289
61	8	0	0.343912	1.063311	-2.851028
62	1	0	-0.631140	1.036786	-2.980787
63	1	0	0.503320	1.890328	-2.345160

E(RTPSSh) = -1616.22327295

Zero-point correction= 0.517993 (Hartree/Particle)

Thermal correction to Energy= 0.549708

Thermal correction to Enthalpy= 0.550652

Thermal correction to Gibbs Free Energy= 0.458034

Sum of electronic and zero-point Energies= -1615.705280

Sum of electronic and thermal Energies= -1615.673565

Sum of electronic and thermal Enthalpies= -1615.672621

Sum of electronic and thermal Free Energies= -1615.765239

F10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.278484	0.840673	1.250299
2	6	0	-3.366547	-0.655091	0.970724
3	7	0	-2.055151	-1.344849	1.134039
4	6	0	-1.705202	-1.453751	2.575814
5	6	0	-0.205802	-1.583207	2.808600
6	7	0	0.621047	-0.492348	2.214043
7	6	0	0.312157	0.827619	2.817775
8	6	0	1.016078	1.992886	2.110974
9	6	0	-2.888413	1.818993	-0.934500
10	6	0	-1.872163	2.105691	-2.052287
11	8	0	-2.199749	2.858240	-2.976318
12	8	0	-0.741526	1.473865	-1.953439
13	6	0	-2.154287	-2.695247	0.524719
14	6	0	-2.230715	-2.636739	-1.012446
15	8	0	-2.623567	-3.629652	-1.629398
16	8	0	-1.826857	-1.514486	-1.539588
17	1	0	-3.589006	2.660676	-0.846370
18	1	0	-3.461238	0.941488	-1.254553
19	1	0	-3.020723	-3.245343	0.917450
20	1	0	-1.255124	-3.263851	0.786901
21	6	0	1.807706	2.609598	-0.127377
22	1	0	1.430728	2.893157	-1.116319
23	1	0	2.286363	3.494920	0.313824
24	6	0	2.818770	1.498336	-0.300051

25	6	0	4.197646	1.728907	-0.354335
26	6	0	5.055715	0.643734	-0.548156
27	6	0	3.137330	-0.796011	-0.569131
28	6	0	4.520843	-0.642372	-0.647873
29	1	0	5.143545	-1.521521	-0.763768
30	1	0	0.162691	-2.515159	2.368256
31	1	0	-0.029544	-1.643636	3.894415
32	1	0	-2.093804	-0.576272	3.095522
33	1	0	-2.203415	-2.324069	3.026391
34	1	0	0.600261	0.844119	3.881555
35	1	0	-0.769006	0.968545	2.777795
36	1	0	0.805888	2.913530	2.672089
37	1	0	2.098029	1.846186	2.153492
38	1	0	-2.996839	1.015402	2.292407
39	1	0	-4.273654	1.289816	1.119730
40	1	0	-4.117819	-1.104203	1.637482
41	1	0	-3.697013	-0.825748	-0.056378
42	1	0	4.585754	2.735667	-0.241088
43	1	0	6.128822	0.799319	-0.597501
44	6	0	-0.425438	3.215479	0.524636
45	6	0	-1.791394	2.763551	1.028023
46	7	0	-2.270708	1.509546	0.382293
47	7	0	0.629427	2.174171	0.675312
48	1	0	-2.509393	3.580974	0.863872
49	1	0	-1.751269	2.600417	2.107668
50	1	0	-0.140168	4.126003	1.073591
51	1	0	-0.479814	3.475995	-0.532782
52	7	0	2.310692	0.258486	-0.423522
53	6	0	2.480948	-2.169582	-0.567129
54	8	0	1.184465	-2.156401	-0.476886
55	8	0	3.203077	-3.172069	-0.635779
56	63	0	-0.207222	-0.165234	-0.377771
57	6	0	2.026672	-0.855684	2.515845
58	1	0	2.249941	-1.827120	2.072154
59	1	0	2.717105	-0.117995	2.110396
60	1	0	2.178961	-0.920148	3.604030

61	8	0	0.422745	-0.976709	-2.810203
62	1	0	0.849382	-1.787383	-2.464363
63	1	0	-0.523014	-1.248068	-2.883369

E(RTPSSh) = -1616.22662546

Zero-point correction= 0.518200 (Hartree/Particle)

Thermal correction to Energy= 0.549864

Thermal correction to Enthalpy= 0.550808

Thermal correction to Gibbs Free Energy= 0.458474

Sum of electronic and zero-point Energies= -1615.708425

Sum of electronic and thermal Energies= -1615.676762

Sum of electronic and thermal Enthalpies= -1615.675817

Sum of electronic and thermal Free Energies= -1615.768151

F11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.647628	-2.210109	0.649376
2	6	0	0.400198	-3.242198	0.396253
3	6	0	1.786396	-2.806320	0.870624
4	7	0	2.255424	-1.525130	0.274082
5	7	0	2.048517	1.323031	1.176570
6	6	0	1.704654	1.351635	2.630726
7	6	0	0.696353	0.273488	3.037956
8	7	0	-0.572904	0.341378	2.268383
9	6	0	-1.452024	-0.809281	2.615306
10	6	0	-0.952265	-2.160968	2.110285
11	6	0	2.855357	-1.773527	-1.062801
12	6	0	1.831976	-2.009140	-2.183954
13	8	0	2.160373	-2.680114	-3.165248
14	8	0	0.684120	-1.411861	-2.022397
15	6	0	2.163175	2.697030	0.619625
16	6	0	2.177359	2.707244	-0.922879
17	8	0	2.571633	3.722871	-1.501794

18	8	0	1.719678	1.628859	-1.493848
19	1	0	3.559253	-2.616028	-1.023449
20	1	0	3.423172	-0.881870	-1.351827
21	1	0	3.054340	3.215199	0.998855
22	1	0	1.283536	3.269335	0.932881
23	1	0	0.411352	-3.443535	-0.675302
24	1	0	0.144837	-4.184099	0.905378
25	1	0	2.495968	-3.617797	0.650425
26	1	0	1.788073	-2.686380	1.957434
27	1	0	2.610246	1.228095	3.239089
28	1	0	1.304727	2.339818	2.868601
29	1	0	1.127909	-0.716989	2.882682
30	1	0	0.495416	0.372279	4.117349
31	1	0	-2.437705	-0.592047	2.200928
32	1	0	-1.569235	-0.879775	3.708665
33	1	0	-0.047110	-2.440911	2.651411
34	1	0	-1.705950	-2.920718	2.363076
35	6	0	-1.859848	-2.567754	-0.137623
36	1	0	-1.518793	-2.829694	-1.145959
37	1	0	-2.356836	-3.452796	0.284580
38	6	0	-2.843706	-1.424061	-0.265908
39	6	0	-4.227967	-1.613012	-0.324916
40	6	0	-3.089687	0.882720	-0.539155
41	6	0	-5.050703	-0.499432	-0.515180
42	1	0	-4.648254	-2.607807	-0.220897
43	6	0	-4.477117	0.769158	-0.626010
44	1	0	-6.128265	-0.621781	-0.564547
45	1	0	-5.072485	1.664057	-0.763595
46	6	0	3.273018	-0.881995	1.154715
47	6	0	3.342238	0.623045	0.929274
48	1	0	3.625966	0.830016	-0.105526
49	1	0	4.124666	1.046587	1.576885
50	1	0	4.269397	-1.314589	0.984460
51	1	0	3.016237	-1.093121	2.195327
52	7	0	-2.302256	-0.197557	-0.373358
53	6	0	-2.378656	2.230304	-0.590377

54	8	0	-1.110596	2.188177	-0.342385
55	8	0	-3.052833	3.240693	-0.838432
56	63	0	0.193924	0.192183	-0.328793
57	6	0	-1.306738	1.577155	2.636959
58	1	0	-2.276702	1.578328	2.138319
59	1	0	-1.463822	1.621741	3.725409
60	1	0	-0.760047	2.462435	2.313134
61	8	0	-0.492184	0.782865	-2.789115
62	1	0	0.273328	1.402214	-2.792341
63	1	0	-0.102132	-0.075475	-3.074600

E(RTPSSh) = -1616.22969113 Zero-point correction= 0.518563 (Hartree/Particle)

Thermal correction to Energy= 0.550016

Thermal correction to Enthalpy= 0.550960

Thermal correction to Gibbs Free Energy= 0.459110

Sum of electronic and zero-point Energies= -1615.711128

Sum of electronic and thermal Energies= -1615.679675

Sum of electronic and thermal Enthalpies= -1615.678731

Sum of electronic and thermal Free Energies= -1615.770581

F12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.413767	-2.119150	0.886442
2	6	0	0.583163	-3.177088	0.537148
3	6	0	2.033245	-2.784180	0.806953
4	7	0	2.427917	-1.488696	0.190776
5	7	0	2.034758	1.254386	1.189688
6	7	0	-0.777498	0.672420	2.221841
7	6	0	-1.178738	-0.642825	2.805454
8	6	0	-0.359285	-1.846767	2.352190
9	6	0	2.945272	-1.708380	-1.180893
10	6	0	1.853918	-2.053124	-2.202727

11	8	0	2.117439	-2.795838	-3.151022
12	8	0	0.708674	-1.459382	-2.002291
13	6	0	2.030468	2.683423	0.789517
14	6	0	2.037917	2.845960	-0.747948
15	8	0	2.380795	3.929968	-1.226392
16	8	0	1.633374	1.804623	-1.418839
17	1	0	3.719364	-2.488490	-1.190483
18	1	0	3.407908	-0.774486	-1.523117
19	1	0	2.881414	3.225686	1.224029
20	1	0	1.113923	3.156400	1.157480
21	1	0	0.447208	-3.398591	-0.521882
22	1	0	0.372390	-4.098683	1.102608
23	1	0	2.674466	-3.600256	0.442042
24	1	0	2.209212	-2.719500	1.882901
25	1	0	-2.226742	-0.804256	2.539752
26	1	0	-1.135642	-0.598336	3.904144
27	1	0	0.686618	-1.691545	2.618706
28	1	0	-0.706736	-2.729397	2.911664
29	6	0	-1.749876	-2.636810	0.478442
30	1	0	-1.595597	-3.275039	-0.398710
31	1	0	-2.171584	-3.282063	1.262648
32	6	0	-2.757884	-1.579232	0.082087
33	6	0	-4.130561	-1.859691	0.059464
34	6	0	-5.011367	-0.881562	-0.401691
35	6	0	-3.136118	0.582484	-0.707325
36	6	0	-4.508639	0.361910	-0.794723
37	1	0	-5.149781	1.165332	-1.137657
38	1	0	-4.493853	-2.825837	0.394590
39	1	0	-6.077926	-1.081133	-0.436415
40	6	0	3.470564	-0.808072	1.003904
41	6	0	3.384627	0.707106	0.871223
42	1	0	3.612575	1.002132	-0.156209
43	1	0	4.140849	1.169490	1.524430
44	1	0	4.479607	-1.129361	0.707650
45	1	0	3.348550	-1.109123	2.046482
46	6	0	0.286667	1.374365	3.007275

47	6	0	1.730278	1.056941	2.630912
48	1	0	0.161208	1.171602	4.081285
49	1	0	0.114990	2.445340	2.872557
50	1	0	1.956438	0.018476	2.876275
51	1	0	2.389546	1.681972	3.253203
52	7	0	-2.282377	-0.383325	-0.300766
53	6	0	-2.524001	1.951930	-0.974466
54	8	0	-3.248241	2.836427	-1.455346
55	8	0	-1.286490	2.069156	-0.624278
56	63	0	0.188013	0.202900	-0.380464
57	6	0	-1.973639	1.555814	2.308356
58	1	0	-1.754211	2.512022	1.833904
59	1	0	-2.813874	1.092532	1.791364
60	1	0	-2.255769	1.722464	3.358993
61	8	0	-0.386192	0.712357	-2.883412
62	1	0	0.317801	1.398543	-2.868547
63	1	0	0.068683	-0.119732	-3.146578

E(RTPSSh) = -1616.21831090

Zero-point correction= 0.518836 (Hartree/Particle)

Thermal correction to Energy= 0.550269

Thermal correction to Enthalpy= 0.551214

Thermal correction to Gibbs Free Energy= 0.459274

Sum of electronic and zero-point Energies= -1615.699475

Sum of electronic and thermal Energies= -1615.668042

Sum of electronic and thermal Enthalpies= -1615.667097

Sum of electronic and thermal Free Energies= -1615.759037

F13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.851777	2.107619	0.668891
2	6	0	-0.171587	3.183417	0.536424
3	6	0	-1.574779	2.789766	1.010493

4	7	0	-2.096972	1.519793	0.421032
5	7	0	-2.047660	-1.480064	0.996765
6	6	0	-1.566155	-1.979813	2.312361
7	6	0	-0.887091	-0.910691	3.158918
8	7	0	0.256887	-0.275833	2.444615
9	6	0	-2.783622	1.804269	-0.867136
10	6	0	-1.828854	2.077407	-2.039660
11	8	0	-2.242806	2.712957	-3.012575
12	8	0	-0.641373	1.552578	-1.923258
13	6	0	-2.385689	-2.648166	0.139279
14	6	0	-2.516893	-2.246181	-1.340855
15	8	0	-3.171705	-2.970378	-2.100052
16	8	0	-1.873325	-1.169985	-1.672936
17	1	0	-3.486329	2.641488	-0.756701
18	1	0	-3.357400	0.916901	-1.152110
19	1	0	-3.305132	-3.143701	0.478726
20	1	0	-1.566737	-3.372139	0.212113
21	1	0	-0.205487	3.458832	-0.517604
22	1	0	0.137313	4.075799	1.102515
23	1	0	-2.252782	3.622266	0.772514
24	1	0	-1.587638	2.691037	2.095886
25	1	0	-2.394423	-2.421976	2.886602
26	1	0	-0.851487	-2.780766	2.099972
27	1	0	-1.601137	-0.136540	3.440100
28	1	0	-0.544600	-1.371174	4.097425
29	6	0	2.010298	2.448504	-0.205696
30	1	0	1.607642	2.689612	-1.195936
31	1	0	2.548472	3.332875	0.163886
32	6	0	2.954894	1.271266	-0.342196
33	6	0	4.338825	1.396795	-0.499239
34	6	0	5.102826	0.238530	-0.668123
35	6	0	3.093334	-1.058223	-0.490407
36	6	0	4.476214	-1.010717	-0.663625
37	1	0	5.028433	-1.935495	-0.782869
38	1	0	4.804664	2.376558	-0.487041
39	1	0	6.178752	0.311728	-0.792590

40	6	0	-3.047086	0.866334	1.366412
41	6	0	-3.271861	-0.623773	1.088554
42	1	0	-3.797112	-0.727710	0.135838
43	1	0	-3.944945	-1.017854	1.864552
44	1	0	-4.030130	1.360799	1.333500
45	1	0	-2.662195	1.015302	2.374774
46	6	0	1.354517	1.955976	2.066566
47	6	0	0.484450	1.092458	2.975921
48	1	0	1.473710	2.945429	2.532305
49	1	0	2.352569	1.513567	2.006495
50	1	0	-0.488702	1.558068	3.129721
51	1	0	0.969258	1.047472	3.964138
52	7	0	2.363361	0.064003	-0.340301
53	6	0	2.310056	-2.366992	-0.449418
54	8	0	1.035283	-2.232961	-0.258922
55	8	0	2.930196	-3.429638	-0.588050
56	63	0	-0.178969	-0.185179	-0.327183
57	6	0	1.465917	-1.104013	2.682662
58	1	0	1.293751	-2.116901	2.317629
59	1	0	2.318921	-0.689317	2.144750
60	1	0	1.701931	-1.137729	3.757135
61	8	0	0.753019	-0.437934	-2.778865
62	1	0	1.697103	-0.256436	-2.930257
63	1	0	0.286387	0.413644	-2.970106

E(RTPSSh) = -1616.22480515

Zero-point correction= 0.518386 (Hartree/Particle)

Thermal correction to Energy= 0.549953

Thermal correction to Enthalpy= 0.550897

Thermal correction to Gibbs Free Energy= 0.459146

Sum of electronic and zero-point Energies= -1615.706419

Sum of electronic and thermal Energies= -1615.674853

Sum of electronic and thermal Enthalpies= -1615.673908

Sum of electronic and thermal Free Energies= -1615.765659

F14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.576029	1.732561	1.353035
2	6	0	-0.362803	2.895056	1.293516
3	6	0	-1.821402	2.474403	1.150776
4	7	0	-2.100228	1.700784	-0.086174
5	6	0	-3.432048	1.046653	-0.011254
6	6	0	-3.526521	0.021030	1.118433
7	7	0	-2.380713	-0.943234	1.162785
8	7	0	0.526868	-1.280422	2.024620
9	6	0	1.173106	-0.220911	2.853490
10	6	0	0.563473	1.173492	2.733853
11	6	0	-2.044900	2.585252	-1.274950
12	6	0	-0.616843	2.799526	-1.808907
13	8	0	-0.379783	3.806595	-2.487316
14	8	0	0.227456	1.856467	-1.527988
15	6	0	-2.800703	-2.228063	0.550289
16	6	0	-2.907787	-2.141450	-0.977359
17	8	0	-3.716597	-2.850649	-1.580211
18	8	0	-2.054062	-1.322326	-1.520999
19	1	0	-2.519967	3.555656	-1.076715
20	1	0	-2.610552	2.101200	-2.079541
21	1	0	-3.749949	-2.579599	0.976551
22	1	0	-2.040772	-2.987768	0.762000
23	1	0	-0.071334	3.524790	0.451614
24	1	0	-0.265847	3.510139	2.200524
25	1	0	-2.451470	3.376998	1.185153
26	1	0	-2.106977	1.861590	2.007333
27	1	0	-4.230759	1.791495	0.133873
28	1	0	-3.596812	0.559761	-0.974397
29	1	0	-4.472518	-0.523924	1.006098
30	1	0	-3.587231	0.528283	2.084438
31	1	0	2.223492	-0.175382	2.557497

32	1	0	1.156432	-0.510370	3.915446
33	1	0	-0.470897	1.166347	3.079492
34	1	0	1.114900	1.842056	3.413688
35	6	0	1.931739	2.218455	0.981559
36	1	0	1.800333	2.918127	0.150670
37	1	0	2.389657	2.771768	1.814216
38	6	0	2.878390	1.151346	0.484863
39	6	0	4.265760	1.295989	0.615527
40	6	0	5.103898	0.342167	0.038178
41	6	0	3.147310	-0.826602	-0.707394
42	6	0	4.536832	-0.739117	-0.639494
43	1	0	5.136398	-1.515663	-1.099553
44	1	0	4.673009	2.143334	1.157368
45	1	0	6.181909	0.437534	0.123091
46	6	0	-0.646080	-1.896608	2.715110
47	6	0	-1.970675	-1.158122	2.576353
48	1	0	-0.428244	-2.013945	3.787708
49	1	0	-0.752513	-2.907133	2.311950
50	1	0	-1.914436	-0.180317	3.057737
51	1	0	-2.735510	-1.732865	3.122302
52	7	0	2.337091	0.105534	-0.162735
53	6	0	2.459527	-2.002868	-1.378732
54	8	0	3.153739	-2.877234	-1.911565
55	8	0	1.161694	-1.978172	-1.322009
56	63	0	-0.226062	-0.169022	-0.456730
57	6	0	1.516044	-2.381830	1.867070
58	1	0	1.110048	-3.141767	1.197375
59	1	0	2.438562	-1.989904	1.439646
60	1	0	1.747908	-2.841600	2.839551
61	8	0	-0.198419	-0.592516	-3.144208
62	1	0	-1.085879	-1.000325	-3.003739
63	1	0	0.417460	-1.330780	-2.939285

E(RTPSSh) = -1616.22076858

Zero-point correction= 0.518956 (Hartree/Particle)

Thermal correction to Energy= 0.550405

Thermal correction to Enthalpy= 0.551349

Thermal correction to Gibbs Free Energy= 0.459578

Sum of electronic and zero-point Energies= -1615.701812

Sum of electronic and thermal Energies= -1615.670364

Sum of electronic and thermal Enthalpies= -1615.669420

Sum of electronic and thermal Free Energies= -1615.761190

F15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.733459	1.762149	1.261666
2	6	0	-0.272822	2.863850	1.359201
3	6	0	-1.728918	2.402876	1.338111
4	7	0	-2.097614	1.656539	0.105854
5	6	0	-3.439597	1.033650	0.256979
6	6	0	-3.459698	-0.101710	1.275432
7	7	0	-2.426143	-1.149477	1.037256
8	7	0	0.385281	-1.159101	2.088098
9	6	0	-2.121709	2.573707	-1.060437
10	6	0	-0.741797	2.787248	-1.701040
11	8	0	-0.504881	3.851950	-2.285195
12	8	0	0.067545	1.776798	-1.613641
13	6	0	-2.946878	-2.183485	0.104780
14	6	0	-2.996634	-1.740976	-1.365552
15	8	0	-3.840781	-2.235679	-2.116512
16	8	0	-2.070691	-0.892752	-1.715082
17	1	0	-2.568354	3.542772	-0.799101
18	1	0	-2.750787	2.115079	-1.831131
19	1	0	-3.941378	-2.527523	0.420060
20	1	0	-2.269377	-3.045672	0.144903
21	1	0	-0.100855	3.547006	0.524231
22	1	0	-0.109571	3.445101	2.277749
23	1	0	-2.369533	3.292863	1.446547
24	1	0	-1.928297	1.764847	2.200407

25	1	0	-4.184800	1.783119	0.567989
26	1	0	-3.733573	0.666444	-0.727087
27	1	0	-4.465305	-0.547343	1.278710
28	1	0	-3.301044	0.303728	2.277221
29	6	0	1.968398	2.324228	0.641796
30	1	0	1.660819	2.887311	-0.243629
31	1	0	2.475377	3.016135	1.329237
32	6	0	2.923611	1.243383	0.192102
33	6	0	4.311600	1.423824	0.196709
34	6	0	5.128760	0.397043	-0.279714
35	6	0	3.154663	-0.908095	-0.669650
36	6	0	4.543658	-0.793818	-0.714861
37	1	0	5.130627	-1.633918	-1.067020
38	1	0	4.737237	2.349410	0.570265
39	1	0	6.207464	0.518262	-0.290931
40	6	0	0.246327	-0.012402	3.021469
41	6	0	1.086523	1.194472	2.602379
42	1	0	0.992354	1.969371	3.375493
43	1	0	2.141392	0.910503	2.571439
44	1	0	-0.804871	0.275852	3.057720
45	1	0	0.536847	-0.306250	4.042699
46	6	0	-0.602042	-2.239016	2.378844
47	6	0	-2.059529	-1.803031	2.328752
48	1	0	-0.410891	-2.668986	3.375308
49	1	0	-0.413910	-3.030552	1.645056
50	1	0	-2.269708	-1.108024	3.144134
51	1	0	-2.688879	-2.684820	2.512010
52	7	0	2.365861	0.100713	-0.247406
53	6	0	2.448534	-2.203010	-1.040262
54	8	0	3.128937	-3.159361	-1.434269
55	8	0	1.158562	-2.185384	-0.889723
56	63	0	-0.196196	-0.198876	-0.402595
57	6	0	1.719369	-1.782029	2.267345
58	1	0	1.810117	-2.625507	1.582186
59	1	0	2.512308	-1.068247	2.050472
60	1	0	1.838761	-2.141923	3.300547

61	8	0	0.205997	-0.804426	-2.966235
62	1	0	-0.771425	-0.929310	-3.017644
63	1	0	0.545263	-1.685685	-2.701665

E(RTPSSh) = -1616.22338370

Zero-point correction= 0.518943 (Hartree/Particle)

Thermal correction to Energy= 0.550338

Thermal correction to Enthalpy= 0.551282

Thermal correction to Gibbs Free Energy= 0.459578

Sum of electronic and zero-point Energies= -1615.704440

Sum of electronic and thermal Energies= -1615.673046

Sum of electronic and thermal Enthalpies= -1615.672101

Sum of electronic and thermal Free Energies= -1615.763806

F16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.754318	1.519023	1.517716
2	6	0	-0.312183	2.503947	1.871331
3	6	0	-1.735671	1.939226	1.900173
4	7	0	-2.181274	1.351012	0.610100
5	6	0	-3.392432	0.507563	0.818895
6	6	0	-3.059018	-0.870259	1.386993
7	7	0	-2.167269	-1.676202	0.510392
8	6	0	-1.589557	-2.837095	1.244577
9	6	0	-0.746708	-2.431893	2.448705
10	7	0	0.331258	-1.461056	2.091423
11	6	0	-2.471057	2.421742	-0.373847
12	6	0	-1.237746	2.945121	-1.121703
13	8	0	-1.277629	4.066018	-1.636582
14	8	0	-0.238586	2.111924	-1.203428
15	6	0	-2.925281	-2.179912	-0.664963
16	6	0	-3.008033	-1.169890	-1.823323
17	8	0	-3.975442	-1.222728	-2.593165

18	8	0	-1.998819	-0.362550	-1.922104
19	1	0	-3.005498	3.261510	0.091611
20	1	0	-3.121002	1.998640	-1.145978
21	1	0	-3.932732	-2.506505	-0.375476
22	1	0	-2.393436	-3.055527	-1.055201
23	1	0	-0.264675	3.314803	1.141616
24	1	0	-0.104235	2.951690	2.854222
25	1	0	-2.412401	2.757555	2.194800
26	1	0	-1.823478	1.171232	2.669317
27	1	0	-4.099461	1.001462	1.502515
28	1	0	-3.898752	0.404072	-0.142815
29	1	0	-3.998264	-1.413188	1.573866
30	1	0	-2.569193	-0.747788	2.353855
31	1	0	-2.383696	-3.521326	1.581657
32	1	0	-0.965115	-3.381502	0.528487
33	1	0	-1.372677	-1.999323	3.232667
34	1	0	-0.310426	-3.341628	2.881383
35	6	0	1.903484	2.258076	0.915639
36	1	0	1.497847	2.907962	0.134716
37	1	0	2.407734	2.886714	1.663253
38	6	0	2.891291	1.306417	0.275662
39	6	0	4.267263	1.553310	0.208230
40	6	0	5.086870	0.623006	-0.435265
41	6	0	3.145835	-0.720942	-0.855695
42	6	0	4.523025	-0.537995	-0.971770
43	1	0	5.119710	-1.299123	-1.460750
44	1	0	4.683891	2.450488	0.654131
45	1	0	6.156653	0.795289	-0.501726
46	6	0	0.443620	-0.420205	3.144568
47	6	0	1.269152	0.786950	2.714949
48	1	0	1.350576	1.476500	3.568111
49	1	0	2.284571	0.456475	2.481089
50	1	0	-0.564429	-0.110419	3.425993
51	1	0	0.907848	-0.838085	4.052886
52	7	0	2.357347	0.195009	-0.258677
53	6	0	2.438243	-1.975124	-1.360754

54	8	0	3.116546	-2.849716	-1.917694
55	8	0	1.163560	-2.005679	-1.138825
56	63	0	-0.182531	-0.151960	-0.431716
57	6	0	1.605969	-2.208328	1.978059
58	1	0	1.498249	-2.985734	1.220923
59	1	0	2.412575	-1.542000	1.671614
60	1	0	1.871403	-2.669709	2.941826
61	8	0	0.722889	0.386946	-2.839441
62	1	0	1.686295	0.368583	-2.975460
63	1	0	0.498386	1.331864	-2.654568

E(RTPSSh) = -1616.22477796

Zero-point correction= 0.517739 (Hartree/Particle)

Thermal correction to Energy= 0.549506

Thermal correction to Enthalpy= 0.550451

Thermal correction to Gibbs Free Energy= 0.458113

Sum of electronic and zero-point Energies= -1615.707039

Sum of electronic and thermal Energies= -1615.675272

Sum of electronic and thermal Enthalpies= -1615.674327

Sum of electronic and thermal Free Energies= -1615.766665

[Gd(1,4-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.665140	1.760088	1.334910
2	6	0	-0.360486	2.845699	1.390896
3	6	0	-1.789284	2.309031	1.467626
4	7	0	-2.185742	1.488690	0.291129
5	6	0	-3.429874	0.728872	0.589166
6	6	0	-3.183183	-0.465400	1.504300
7	7	0	-2.198660	-1.445333	0.966683

8	6	0	-1.648159	-2.248177	2.097338
9	6	0	-0.598750	-1.477352	2.897300
10	7	0	0.623540	-1.179178	2.104505
11	6	0	1.455343	-0.158705	2.796356
12	6	0	0.884719	1.252518	2.720697
13	6	0	-2.408440	2.361078	-0.885713
14	6	0	-1.112607	2.764682	-1.600760
15	8	0	-1.079490	3.811563	-2.254075
16	8	0	-0.138912	1.903678	-1.499454
17	6	0	-2.849373	-2.326218	-0.037286
18	6	0	-2.922127	-1.714040	-1.449143
19	8	0	-3.828721	-2.065398	-2.208649
20	8	0	-1.952532	-0.897368	-1.750088
21	1	0	-2.985105	3.257955	-0.620804
22	1	0	-2.990227	1.790450	-1.617523
23	1	0	-3.853869	-2.628662	0.286218
24	1	0	-2.243861	-3.234715	-0.132506
25	1	0	-0.241739	3.473145	0.506897
26	1	0	-0.185308	3.490603	2.264538
27	1	0	-2.474435	3.164192	1.578505
28	1	0	-1.907542	1.695804	2.364466
29	1	0	-4.184000	1.378753	1.059298
30	1	0	-3.844747	0.390948	-0.362934
31	1	0	-4.143264	-0.968766	1.692507
32	1	0	-2.819932	-0.119222	2.474268
33	1	0	-2.453524	-2.565847	2.775953
34	1	0	-1.206719	-3.155042	1.677240
35	1	0	-1.019111	-0.533761	3.252747
36	1	0	-0.334238	-2.062442	3.792157
37	1	0	2.448058	-0.187788	2.342387
38	1	0	1.579571	-0.423044	3.858852
39	1	0	-0.075774	1.288441	3.239623
40	1	0	1.557204	1.930839	3.266715
41	6	0	1.921533	2.320145	0.761944
42	1	0	1.628788	2.951268	-0.083257
43	1	0	2.437323	2.956480	1.495099

44	6	0	2.870457	1.272437	0.220849
45	6	0	4.256511	1.462813	0.188078
46	6	0	3.077574	-0.794997	-0.845332
47	6	0	5.057048	0.487469	-0.410821
48	1	0	4.694718	2.355300	0.622535
49	6	0	4.462298	-0.661156	-0.938377
50	1	0	6.134068	0.617889	-0.452256
51	1	0	5.039669	-1.453633	-1.399987
52	7	0	2.308066	0.164399	-0.292499
53	6	0	2.347683	-2.048373	-1.315790
54	8	0	2.994209	-2.907954	-1.933449
55	8	0	1.100112	-2.102695	-0.987991
56	6	0	1.437270	-2.415493	2.003571
57	1	0	2.353755	-2.199031	1.454317
58	1	0	1.698530	-2.786571	3.006692
59	1	0	0.892361	-3.188990	1.462910
60	8	0	0.337057	-0.190150	-2.958181
61	1	0	0.212860	0.786186	-2.932902
62	1	0	-0.569528	-0.546895	-3.089355
63	64	0	-0.185829	-0.193389	-0.356403

E(RTPSSh) = -1616.82187655

Zero-point correction= 0.518497 (Hartree/Particle)

Thermal correction to Energy= 0.549956

Thermal correction to Enthalpy= 0.550900

Thermal correction to Gibbs Free Energy= 0.459199

Sum of electronic and zero-point Energies= -1616.303380

Sum of electronic and thermal Energies= -1616.271921

Sum of electronic and thermal Enthalpies= -1616.270977

Sum of electronic and thermal Free Energies= -1616.362677

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	0.804493	1.649952	1.485769
2	6	0	-0.219614	2.655120	1.880543
3	6	0	-1.148771	3.041332	0.740355
4	7	0	-1.869158	1.877820	0.157181
5	6	0	-3.023739	1.490347	1.000345
6	6	0	-3.528389	0.091559	0.660376
7	7	0	-2.491330	-0.964359	0.839445
8	6	0	-2.365886	-1.311222	2.281065
9	6	0	-1.049414	-2.008376	2.608940
10	7	0	0.158498	-1.207160	2.264446
11	6	0	0.330880	-0.085575	3.223460
12	6	0	1.306789	0.970083	2.713875
13	6	0	-2.298627	2.253875	-1.205866
14	6	0	-1.093010	2.336414	-2.152831
15	8	0	-1.201164	2.935327	-3.225835
16	8	0	-0.025760	1.706711	-1.738303
17	6	0	-2.904595	-2.149322	0.046027
18	6	0	-2.703828	-1.929660	-1.466167
19	8	0	-3.354371	-2.609535	-2.262703
20	8	0	-1.800865	-1.041453	-1.780938
21	1	0	-2.845946	3.207587	-1.212656
22	1	0	-2.967216	1.483250	-1.600679
23	1	0	-3.950229	-2.419196	0.246683
24	1	0	-2.282724	-3.003759	0.335872
25	6	0	1.932127	2.316500	0.783554
26	1	0	1.510769	2.918611	-0.028147
27	1	0	2.474783	2.993218	1.460074
28	6	0	2.883381	1.297607	0.189899
29	6	0	4.251080	1.533128	0.018431
30	6	0	3.088420	-0.860364	-0.683810
31	6	0	5.039251	0.527855	-0.548363
32	1	0	4.687085	2.477274	0.328141
33	6	0	4.455570	-0.692244	-0.899680
34	1	0	6.102789	0.690006	-0.694460
35	1	0	5.030880	-1.509674	-1.318343
36	1	0	-0.975528	-2.946380	2.050395

37	1	0	-1.044208	-2.270567	3.678491
38	1	0	-2.459422	-0.388123	2.857859
39	1	0	-3.197190	-1.960871	2.592622
40	1	0	0.689079	-0.467444	4.192146
41	1	0	-0.646000	0.366911	3.406982
42	1	0	1.489768	1.708887	3.508371
43	1	0	2.269124	0.510381	2.478642
44	1	0	0.264649	3.561804	2.273279
45	1	0	-0.798919	2.231433	2.703648
46	1	0	-0.571721	3.506849	-0.061400
47	1	0	-1.865441	3.794877	1.100957
48	1	0	-2.709268	1.534214	2.046883
49	1	0	-3.852457	2.206513	0.889061
50	1	0	-4.411210	-0.137862	1.275258
51	1	0	-3.851747	0.057806	-0.383228
52	7	0	2.329868	0.127104	-0.170762
53	6	0	2.363076	-2.171917	-0.960180
54	8	0	3.003067	-3.101809	-1.473660
55	8	0	1.125215	-2.193219	-0.590094
56	8	0	0.643375	-0.541214	-2.820157
57	1	0	0.523089	0.435183	-2.900237
58	1	0	-0.252465	-0.908079	-2.990113
59	6	0	1.330431	-2.111272	2.380341
60	1	0	1.211874	-2.941666	1.685836
61	1	0	2.243998	-1.576122	2.117134
62	1	0	1.421057	-2.492034	3.409161
63	64	0	-0.167979	-0.210128	-0.281393

E(RTPSSh) = -1616.82348987

Zero-point correction= 0.518810 (Hartree/Particle)

Thermal correction to Energy= 0.550034

Thermal correction to Enthalpy= 0.550978

Thermal correction to Gibbs Free Energy= 0.460172

Sum of electronic and zero-point Energies= -1616.304680

Sum of electronic and thermal Energies= -1616.273456

Sum of electronic and thermal Enthalpies= -1616.272512

Sum of electronic and thermal Free Energies= -1616.363318

[Ho(1,4-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.632566	1.798401	1.317165
2	6	0	-0.431723	2.843830	1.398206
3	6	0	-1.830975	2.238546	1.521877
4	7	0	-2.221973	1.405552	0.351775
5	6	0	-3.408811	0.568849	0.675141
6	6	0	-3.056975	-0.626421	1.552778
7	7	0	-2.015001	-1.524500	0.970327
8	6	0	-1.415630	-2.327097	2.077439
9	6	0	-0.408601	-1.517916	2.889290
10	7	0	0.773453	-1.125400	2.078418
11	6	0	1.552884	-0.064524	2.769256
12	6	0	0.905326	1.311597	2.700232
13	6	0	-2.522061	2.269843	-0.814718
14	6	0	-1.269977	2.716629	-1.579752
15	8	0	-1.310557	3.741366	-2.266348
16	8	0	-0.249145	1.912111	-1.476734
17	6	0	-2.624343	-2.427527	-0.042551
18	6	0	-2.788813	-1.783490	-1.429834
19	8	0	-3.675875	-2.193191	-2.182716
20	8	0	-1.904019	-0.872304	-1.719353
21	1	0	-3.117996	3.146128	-0.525638
22	1	0	-3.112423	1.680409	-1.524022
23	1	0	-3.588386	-2.822321	0.303139
24	1	0	-1.947041	-3.277589	-0.182623
25	1	0	-0.367195	3.469757	0.507614
26	1	0	-0.258747	3.500470	2.263240

27	1	0	-2.554538	3.056779	1.660544
28	1	0	-1.888909	1.613615	2.416376
29	1	0	-4.182546	1.161920	1.185647
30	1	0	-3.835513	0.226699	-0.269812
31	1	0	-3.972716	-1.203381	1.748492
32	1	0	-2.695926	-0.278842	2.522910
33	1	0	-2.201491	-2.707785	2.745758
34	1	0	-0.924430	-3.194868	1.631287
35	1	0	-0.879795	-0.613261	3.281936
36	1	0	-0.091722	-2.111629	3.761014
37	1	0	2.542762	-0.038127	2.308596
38	1	0	1.700414	-0.323810	3.829958
39	1	0	-0.046607	1.295717	3.235732
40	1	0	1.547874	2.029767	3.231059
41	6	0	1.858415	2.379558	0.698950
42	1	0	1.526069	3.006132	-0.134750
43	1	0	2.393104	3.021679	1.413040
44	6	0	2.797157	1.335537	0.127628
45	6	0	4.180447	1.525254	0.034769
46	6	0	2.963943	-0.760712	-0.899761
47	6	0	4.955835	0.533714	-0.571624
48	1	0	4.636857	2.426072	0.431607
49	6	0	4.344222	-0.630042	-1.046425
50	1	0	6.030506	0.662347	-0.656875
51	1	0	4.907850	-1.434334	-1.504598
52	7	0	2.221450	0.216347	-0.342776
53	6	0	2.208384	-2.026464	-1.296861
54	8	0	2.826338	-2.913102	-1.903306
55	8	0	0.971647	-2.064928	-0.917607
56	6	0	1.664424	-2.305290	1.959184
57	1	0	2.555124	-2.030633	1.393089
58	1	0	1.971349	-2.654497	2.957436
59	1	0	1.160440	-3.113395	1.430974
60	8	0	0.407802	-0.151710	-2.870024
61	1	0	0.226053	0.816142	-2.867910
62	1	0	-0.471576	-0.560388	-3.027090

63	67	0	-0.199442	-0.139265	-0.325987

E(RTPSSh) = -1618.58069245

Zero-point correction= 0.518961 (Hartree/Particle)

Thermal correction to Energy= 0.550133

Thermal correction to Enthalpy= 0.551077

Thermal correction to Gibbs Free Energy= 0.460349

Sum of electronic and zero-point Energies= -1618.061731

Sum of electronic and thermal Energies= -1618.030559

Sum of electronic and thermal Enthalpies= -1618.029615

Sum of electronic and thermal Free Energies= -1618.120344

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.770973	1.665411	1.474763
2	6	0	-0.263937	2.658805	1.874291
3	6	0	-1.212422	3.018748	0.741886
4	7	0	-1.901376	1.832555	0.164522
5	6	0	-3.045343	1.416437	1.008527
6	6	0	-3.508100	0.005099	0.664552
7	7	0	-2.432961	-1.015168	0.833391
8	6	0	-2.309127	-1.379499	2.270547
9	6	0	-0.974074	-2.040327	2.591232
10	7	0	0.204138	-1.197357	2.247546
11	6	0	0.342503	-0.077802	3.214061
12	6	0	1.290932	1.002339	2.706071
13	6	0	-2.337693	2.189287	-1.202019
14	6	0	-1.125229	2.306872	-2.134545
15	8	0	-1.232388	2.900593	-3.209699
16	8	0	-0.046462	1.708916	-1.700155
17	6	0	-2.799517	-2.201668	0.020520
18	6	0	-2.581907	-1.951792	-1.482685
19	8	0	-3.186034	-2.643481	-2.304116

20	8	0	-1.713224	-1.017968	-1.762769
21	1	0	-2.915676	3.124383	-1.215676
22	1	0	-2.975302	1.393985	-1.598938
23	1	0	-3.839191	-2.505565	0.201975
24	1	0	-2.157001	-3.041515	0.307721
25	6	0	1.890335	2.339641	0.763747
26	1	0	1.461051	2.935938	-0.047741
27	1	0	2.433292	3.019898	1.435875
28	6	0	2.839515	1.318148	0.170448
29	6	0	4.206851	1.544631	-0.014051
30	6	0	3.026659	-0.851604	-0.683596
31	6	0	4.985237	0.527064	-0.573058
32	1	0	4.650502	2.490031	0.280377
33	6	0	4.393564	-0.694649	-0.906334
34	1	0	6.048768	0.681276	-0.727448
35	1	0	4.963055	-1.519820	-1.317714
36	1	0	-0.872262	-2.970899	2.024962
37	1	0	-0.957052	-2.309884	3.658777
38	1	0	-2.432467	-0.467556	2.859336
39	1	0	-3.123442	-2.057068	2.566343
40	1	0	0.709544	-0.453708	4.181693
41	1	0	-0.645801	0.349242	3.397906
42	1	0	1.454316	1.748631	3.497314
43	1	0	2.264802	0.566825	2.472914
44	1	0	0.210666	3.575733	2.253860
45	1	0	-0.826206	2.231522	2.707567
46	1	0	-0.654441	3.500396	-0.063521
47	1	0	-1.948912	3.750132	1.106972
48	1	0	-2.730388	1.466815	2.054759
49	1	0	-3.892454	2.110521	0.898088
50	1	0	-4.377870	-0.257830	1.284081
51	1	0	-3.837875	-0.034162	-0.376773
52	7	0	2.279675	0.146486	-0.175104
53	6	0	2.284104	-2.155838	-0.946022
54	8	0	2.912565	-3.104475	-1.437294
55	8	0	1.041418	-2.151833	-0.587074

56	8	0	0.720621	-0.491399	-2.789875
57	1	0	0.571194	0.480974	-2.856258
58	1	0	-0.170291	-0.878478	-2.937956
59	6	0	1.404954	-2.063513	2.359158
60	1	0	1.306740	-2.900318	1.669538
61	1	0	2.300589	-1.501447	2.090507
62	1	0	1.512819	-2.437709	3.388624
63	67	0	-0.164025	-0.166850	-0.258828

E(RTPSSh) = -1618.58072825

Zero-point correction= 0.518868 (Hartree/Particle)

Thermal correction to Energy= 0.550120

Thermal correction to Enthalpy= 0.551064

Thermal correction to Gibbs Free Energy= 0.459965

Sum of electronic and zero-point Energies= -1618.061860

Sum of electronic and thermal Energies= -1618.030609

Sum of electronic and thermal Enthalpies= -1618.029664

Sum of electronic and thermal Free Energies= -1618.120763

[Yb(1,4-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.593552	1.801060	1.325492
2	6	0	-0.479150	2.838681	1.404336
3	6	0	-1.874024	2.222921	1.524843
4	7	0	-2.236194	1.350536	0.375099
5	6	0	-3.394898	0.483296	0.720623
6	6	0	-2.989458	-0.705640	1.584078
7	7	0	-1.931081	-1.560858	0.968882
8	6	0	-1.301805	-2.383278	2.043802
9	6	0	-0.314713	-1.576429	2.881012
10	7	0	0.842429	-1.112708	2.073043
11	6	0	1.572416	-0.027632	2.777421

12	6	0	0.866011	1.318651	2.709662
13	6	0	-2.566076	2.179304	-0.809375
14	6	0	-1.325656	2.665380	-1.566838
15	8	0	-1.394927	3.678369	-2.268147
16	8	0	-0.276979	1.900596	-1.439985
17	6	0	-2.525435	-2.451387	-0.064342
18	6	0	-2.715142	-1.775370	-1.431877
19	8	0	-3.589107	-2.193266	-2.195460
20	8	0	-1.863926	-0.825209	-1.696747
21	1	0	-3.203675	3.032514	-0.541391
22	1	0	-3.118733	1.548665	-1.513337
23	1	0	-3.476374	-2.880204	0.277013
24	1	0	-1.826185	-3.278115	-0.232031
25	1	0	-0.417072	3.464471	0.513687
26	1	0	-0.312903	3.496437	2.269870
27	1	0	-2.607538	3.037180	1.628365
28	1	0	-1.940752	1.624200	2.436375
29	1	0	-4.171445	1.055091	1.249985
30	1	0	-3.835318	0.133567	-0.215063
31	1	0	-3.881416	-1.314101	1.794016
32	1	0	-2.617763	-0.352824	2.548633
33	1	0	-2.072665	-2.814098	2.698908
34	1	0	-0.784391	-3.215548	1.560969
35	1	0	-0.808594	-0.706192	3.320087
36	1	0	0.031118	-2.197228	3.722311
37	1	0	2.564288	0.044114	2.324963
38	1	0	1.723666	-0.287082	3.837446
39	1	0	-0.093550	1.255604	3.228229
40	1	0	1.467608	2.061276	3.254766
41	6	0	1.818029	2.394945	0.714056
42	1	0	1.483358	3.039261	-0.104865
43	1	0	2.355670	3.021886	1.439141
44	6	0	2.753056	1.362526	0.115787
45	6	0	4.133287	1.559756	-0.005946
46	6	0	2.908034	-0.727024	-0.929582
47	6	0	4.899072	0.576205	-0.636982

48	1	0	4.594643	2.459607	0.387349
49	6	0	4.283568	-0.588427	-1.106100
50	1	0	5.970902	0.710959	-0.745406
51	1	0	4.842183	-1.386505	-1.581058
52	7	0	2.174721	0.244097	-0.350624
53	6	0	2.144686	-1.993798	-1.306895
54	8	0	2.747852	-2.884257	-1.921570
55	8	0	0.915815	-2.030660	-0.898869
56	6	0	1.784888	-2.248161	1.930658
57	1	0	2.650892	-1.931841	1.347704
58	1	0	2.128993	-2.586154	2.920550
59	1	0	1.306537	-3.077170	1.410993
60	8	0	0.451022	-0.119655	-2.847893
61	1	0	0.258558	0.845668	-2.830072
62	1	0	-0.427538	-0.532225	-2.997563
63	70	0	-0.198066	-0.118294	-0.304207

E(RTPSSh) = -1620.32730524

Zero-point correction= 0.519337 (Hartree/Particle)

Thermal correction to Energy= 0.550396

Thermal correction to Enthalpy= 0.551340

Thermal correction to Gibbs Free Energy= 0.461004

Sum of electronic and zero-point Energies= -1619.807968

Sum of electronic and thermal Energies= -1619.776909

Sum of electronic and thermal Enthalpies= -1619.775965

Sum of electronic and thermal Free Energies= -1619.866301

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.846229	-2.107772	0.755425
2	6	0	-0.148945	-2.906552	1.521523
3	6	0	-1.027217	-2.032406	2.406123
4	7	0	-1.745439	-0.980060	1.634697

5	6	0	-2.957715	-1.539313	0.984249
6	6	0	-3.477295	-0.628745	-0.122535
7	7	0	-2.458045	-0.352376	-1.177723
8	6	0	-2.387090	-1.481173	-2.144068
9	6	0	-1.092948	-1.465821	-2.953163
10	7	0	0.135032	-1.503252	-2.105393
11	6	0	0.347412	-2.877993	-1.574968
12	6	0	1.331489	-2.903313	-0.411218
13	6	0	-2.072150	0.123971	2.566097
14	6	0	-0.805149	0.915867	2.928967
15	8	0	-0.777555	1.578940	3.967574
16	8	0	0.161905	0.850141	2.049440
17	6	0	-2.831002	0.915050	-1.855286
18	6	0	-2.531621	2.130424	-0.960890
19	8	0	-3.083275	3.207134	-1.193224
20	8	0	-1.660239	1.905745	-0.015663
21	1	0	-2.560993	-0.245679	3.477360
22	1	0	-2.753258	0.822432	2.070943
23	1	0	-3.888651	0.915437	-2.150166
24	1	0	-2.234716	1.022126	-2.767604
25	6	0	2.004893	-1.765897	1.623838
26	1	0	1.619183	-1.339123	2.555241
27	1	0	2.583166	-2.664852	1.879846
28	6	0	2.889500	-0.735846	0.955438
29	6	0	4.262768	-0.621147	1.193197
30	6	0	2.944751	1.057598	-0.537819
31	6	0	4.976786	0.384915	0.536628
32	1	0	4.759563	-1.306459	1.871881
33	6	0	4.313237	1.238098	-0.349328
34	1	0	6.043567	0.492202	0.706418
35	1	0	4.827206	2.022649	-0.892311
36	1	0	-1.037027	-0.552374	-3.552207
37	1	0	-1.098750	-2.311157	-3.657045
38	1	0	-2.472021	-2.411537	-1.577115
39	1	0	-3.241125	-1.452909	-2.835856
40	1	0	0.718519	-3.537432	-2.373514

41	1	0	-0.618008	-3.279425	-1.257622
42	1	0	1.514399	-3.944780	-0.110491
43	1	0	2.291901	-2.488210	-0.725034
44	1	0	0.356107	-3.662521	2.140114
45	1	0	-0.764730	-3.450654	0.801463
46	1	0	-0.412965	-1.528792	3.157140
47	1	0	-1.742375	-2.664869	2.951242
48	1	0	-2.697998	-2.520300	0.576367
49	1	0	-3.757895	-1.703187	1.720991
50	1	0	-4.376253	-1.074165	-0.571553
51	1	0	-3.775350	0.333122	0.301294
52	7	0	2.260361	0.095588	0.109232
53	6	0	2.114063	1.899605	-1.491935
54	8	0	2.669372	2.775331	-2.164791
55	8	0	0.851910	1.591882	-1.509424
56	8	0	0.001344	3.720599	1.374735
57	1	0	0.341133	2.954451	1.876567
58	1	0	-0.681838	3.279309	0.820536
59	6	0	1.286192	-1.134953	-2.968978
60	1	0	1.134097	-0.127524	-3.356445
61	1	0	2.208805	-1.146920	-2.387057
62	1	0	1.382699	-1.842167	-3.805769
63	70	0	-0.186869	0.155372	-0.079224

E(RTPSSh) = -1620.33218924

Zero-point correction= 0.518281 (Hartree/Particle)

Thermal correction to Energy= 0.550029

Thermal correction to Enthalpy= 0.550973

Thermal correction to Gibbs Free Energy= 0.458556

Sum of electronic and zero-point Energies= -1619.813908

Sum of electronic and thermal Energies= -1619.782161

Sum of electronic and thermal Enthalpies= -1619.781216

Sum of electronic and thermal Free Energies= -1619.873633

[Lu(1,4-Medo2ampa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.584580	1.800428	1.327720
2	6	0	-0.487010	2.839761	1.401604
3	6	0	-1.881453	2.224142	1.519439
4	7	0	-2.233616	1.343491	0.373161
5	6	0	-3.390729	0.473801	0.719206
6	6	0	-2.981762	-0.712270	1.584701
7	7	0	-1.917070	-1.560764	0.971204
8	6	0	-1.287019	-2.384710	2.043923
9	6	0	-0.304859	-1.575994	2.883811
10	7	0	0.849103	-1.103545	2.077154
11	6	0	1.570847	-0.015839	2.784674
12	6	0	0.853485	1.323589	2.714322
13	6	0	-2.563411	2.165485	-0.816279
14	6	0	-1.322239	2.648890	-1.573284
15	8	0	-1.391859	3.653743	-2.285860
16	8	0	-0.270823	1.889768	-1.433181
17	6	0	-2.504341	-2.450915	-0.066648
18	6	0	-2.693506	-1.771670	-1.432163
19	8	0	-3.558754	-2.194924	-2.202461
20	8	0	-1.850508	-0.811694	-1.688735
21	1	0	-3.202875	3.018793	-0.553408
22	1	0	-3.113626	1.530599	-1.517990
23	1	0	-3.453893	-2.885565	0.271038
24	1	0	-1.800250	-3.273079	-0.235614
25	1	0	-0.422433	3.463124	0.509491
26	1	0	-0.322026	3.499406	2.265867
27	1	0	-2.617081	3.037548	1.613165
28	1	0	-1.952430	1.631164	2.434378
29	1	0	-4.168860	1.044616	1.247018
30	1	0	-3.829863	0.121250	-0.215891

31	1	0	-3.870688	-1.325819	1.792505
32	1	0	-2.614150	-0.357162	2.550134
33	1	0	-2.057211	-2.820875	2.696171
34	1	0	-0.765113	-3.212768	1.558768
35	1	0	-0.803498	-0.710097	3.326053
36	1	0	0.044434	-2.197542	3.723171
37	1	0	2.563260	0.063872	2.334508
38	1	0	1.721588	-0.275414	3.844689
39	1	0	-0.108187	1.252858	3.227909
40	1	0	1.445867	2.072418	3.260986
41	6	0	1.810878	2.394418	0.718851
42	1	0	1.478000	3.043534	-0.096890
43	1	0	2.349712	3.016811	1.446857
44	6	0	2.743112	1.362995	0.115187
45	6	0	4.122488	1.560750	-0.015816
46	6	0	2.892034	-0.726756	-0.930771
47	6	0	4.884112	0.577522	-0.652233
48	1	0	4.586142	2.460918	0.374037
49	6	0	4.266118	-0.587862	-1.116676
50	1	0	5.955016	0.713003	-0.768555
51	1	0	4.822131	-1.385680	-1.595111
52	7	0	2.162418	0.244656	-0.347651
53	6	0	2.124146	-1.992545	-1.300311
54	8	0	2.720582	-2.886563	-1.915890
55	8	0	0.897292	-2.024869	-0.884324
56	6	0	1.798845	-2.232665	1.933344
57	1	0	2.662647	-1.910079	1.350485
58	1	0	2.145779	-2.569024	2.922769
59	1	0	1.325601	-3.064369	1.413428
60	8	0	0.464242	-0.124110	-2.845233
61	1	0	0.274946	0.841578	-2.820723
62	1	0	-0.417864	-0.532775	-2.984688
63	71	0	-0.196518	-0.113981	-0.299007

E(RTPSSh) = -1620.88165935

Zero-point correction= 0.519506 (Hartree/Particle)

Thermal correction to Energy= 0.550534

Thermal correction to Enthalpy= 0.551478

Thermal correction to Gibbs Free Energy= 0.461175

Sum of electronic and zero-point Energies= -1620.362153

Sum of electronic and thermal Energies= -1620.331126

Sum of electronic and thermal Enthalpies= -1620.330182

Sum of electronic and thermal Free Energies= -1620.420485

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.822915	-2.149444	0.659094
2	6	0	-0.177256	-2.967006	1.398278
3	6	0	-1.034808	-2.118905	2.326160
4	7	0	-1.740277	-1.025991	1.601402
5	6	0	-2.962922	-1.543728	0.934944
6	6	0	-3.475456	-0.584272	-0.132874
7	7	0	-2.454341	-0.282644	-1.180497
8	6	0	-2.413001	-1.368493	-2.195229
9	6	0	-1.122726	-1.331312	-3.006519
10	7	0	0.100738	-1.413801	-2.156835
11	6	0	0.301313	-2.815276	-1.694178
12	6	0	1.291862	-2.903856	-0.540315
13	6	0	-2.045237	0.045302	2.578266
14	6	0	-0.763329	0.803088	2.960946
15	8	0	-0.710513	1.413146	4.029929
16	8	0	0.189827	0.769179	2.063038
17	6	0	-2.804141	1.019606	-1.802420
18	6	0	-2.480517	2.190517	-0.859241
19	8	0	-2.991992	3.292654	-1.061416
20	8	0	-1.635042	1.902017	0.092397
21	1	0	-2.532688	-0.353483	3.477679
22	1	0	-2.717684	0.773425	2.115258
23	1	0	-3.862256	1.051832	-2.093808

24	1	0	-2.209188	1.154946	-2.711609
25	6	0	1.992606	-1.855402	1.530123
26	1	0	1.620387	-1.466440	2.482913
27	1	0	2.565827	-2.769085	1.741024
28	6	0	2.877973	-0.804458	0.896692
29	6	0	4.254951	-0.712223	1.122129
30	6	0	2.930116	1.059439	-0.507276
31	6	0	4.969744	0.318077	0.505397
32	1	0	4.753828	-1.432892	1.761448
33	6	0	4.302332	1.219466	-0.328405
34	1	0	6.039511	0.408157	0.666104
35	1	0	4.815708	2.026210	-0.838435
36	1	0	-1.058926	-0.395332	-3.568735
37	1	0	-1.133373	-2.147760	-3.743431
38	1	0	-2.507845	-2.322359	-1.669758
39	1	0	-3.271662	-1.295427	-2.877757
40	1	0	0.660107	-3.438799	-2.526437
41	1	0	-0.665953	-3.222094	-1.389772
42	1	0	1.460829	-3.959118	-0.283183
43	1	0	2.256880	-2.489984	-0.841614
44	1	0	0.321000	-3.757467	1.977959
45	1	0	-0.807529	-3.468489	0.660053
46	1	0	-0.408590	-1.656587	3.093493
47	1	0	-1.756619	-2.761996	2.849430
48	1	0	-2.715652	-2.509705	0.486205
49	1	0	-3.761211	-1.727796	1.668677
50	1	0	-4.380567	-1.001166	-0.596269
51	1	0	-3.760413	0.364091	0.328256
52	7	0	2.245481	0.070911	0.098334
53	6	0	2.093244	1.957646	-1.401937
54	8	0	2.645917	2.857586	-2.043662
55	8	0	0.825915	1.669840	-1.404316
56	8	0	0.099621	3.632213	1.500037
57	1	0	0.439781	2.833163	1.948184
58	1	0	-0.596754	3.229251	0.933391
59	6	0	1.256449	-1.013679	-3.001547

60	1	0	1.112178	0.012537	-3.339865
61	1	0	2.178740	-1.061398	-2.421336
62	1	0	1.346930	-1.679833	-3.871767
63	71	0	-0.191316	0.152255	-0.065814

E(RTPSSh) = -1620.88591814

Zero-point correction= 0.518020 (Hartree/Particle)

Thermal correction to Energy= 0.549900

Thermal correction to Enthalpy= 0.550844

Thermal correction to Gibbs Free Energy= 0.457843

Sum of electronic and zero-point Energies= -1620.367898

Sum of electronic and thermal Energies= -1620.336019

Sum of electronic and thermal Enthalpies= -1620.335074

Sum of electronic and thermal Free Energies= -1620.428075

Complejos de H_2DODPA

Las geometrías optimizadas en disolución se corresponden con las siguientes conformaciones:

- F1: Λ(λλλλ)
- F2: Δ(λλλλ)
- F3: Λ(δλδλ)
- F4: Λ(λδλδ)

[La(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	0.000651	-0.129106	-0.008532
2	7	0	1.968597	1.683842	1.107240
3	6	0	1.354387	2.651340	2.060542
4	6	0	0.070794	2.123176	2.701862
5	6	0	-1.662303	2.919249	1.083650
6	6	0	-2.636031	2.425073	0.012070
7	7	0	-1.962945	1.694709	-1.101630
8	6	0	-1.350028	2.666616	-2.051440
9	6	0	-0.065182	2.144803	-2.696086
10	6	0	1.672171	2.924233	-1.071611
11	6	0	2.643605	2.417875	-0.002865
12	6	0	2.960414	0.824440	1.814928
13	6	0	-2.956020	0.835428	-1.807666
14	8	0	-0.070364	-2.768118	-0.084518
15	1	0	1.131562	3.569013	1.507937
16	1	0	2.071622	2.929979	2.846510
17	1	0	0.267416	1.204627	3.264811
18	1	0	-0.302768	2.871638	3.417285
19	1	0	-0.928019	3.607457	0.651245
20	1	0	-2.228834	3.489969	1.835674
21	1	0	-3.346732	1.738676	0.480296
22	1	0	-3.215151	3.275210	-0.379801
23	1	0	-1.128281	3.581945	-1.494446

24	1	0	-2.067887	2.947798	-2.835910
25	1	0	-0.261067	1.231448	-3.267831
26	1	0	0.307648	2.899745	-3.405074
27	1	0	0.940666	3.612740	-0.634953
28	1	0	2.242288	3.498152	-1.818526
29	1	0	3.350449	1.730601	-0.475844
30	1	0	3.227342	3.262917	0.393356
31	1	0	3.803459	1.423651	2.193602
32	1	0	2.459690	0.387068	2.688465
33	1	0	-3.799295	1.434519	-2.185926
34	1	0	-2.456711	0.396896	-2.681546
35	1	0	0.261362	-3.310836	-0.830775
36	1	0	-0.306662	-3.362527	0.654367
37	6	0	3.474028	-0.282142	0.909459
38	6	0	4.754080	-0.832756	0.998146
39	6	0	5.105278	-1.855015	0.107423
40	1	0	5.460000	-0.476015	1.741826
41	6	0	2.946876	-1.653034	-0.910048
42	6	0	4.191428	-2.282420	-0.858732
43	1	0	6.091622	-2.305586	0.164775
44	1	0	4.418587	-3.073423	-1.564511
45	6	0	-3.468512	-0.269942	-0.899223
46	6	0	-4.748440	-0.820825	-0.986617
47	6	0	-2.937800	-1.640380	0.919764
48	6	0	-5.099417	-1.840588	-0.092941
49	1	0	-5.454431	-0.465964	-1.731151
50	6	0	-4.184590	-2.265926	0.872995
51	1	0	-6.086126	-2.290665	-0.148147
52	1	0	-4.410129	-3.054171	1.582349
53	7	0	-2.597323	-0.683884	0.036044
54	7	0	2.604135	-0.696734	-0.026473
55	6	0	1.842602	-2.013572	-1.901675
56	8	0	0.966219	-1.067330	-2.076327
57	8	0	1.817153	-3.156902	-2.362679
58	6	0	-1.839430	-2.010379	1.916940
59	8	0	-1.868620	-3.127242	2.432732

60	8	0	-0.921431	-1.093780	2.050982
61	7	0	-0.941513	1.782447	1.679090
62	7	0	0.947229	1.795349	-1.676487
63	1	0	-1.610586	1.138760	2.111040
64	1	0	1.613462	1.150764	-2.112046

E(RTPSSh) = -1592.88091767

Zero-point correction= 0.527956 (Hartree/Particle)

Thermal correction to Energy= 0.559720

Thermal correction to Enthalpy= 0.560664

Thermal correction to Gibbs Free Energy= 0.467654

Sum of electronic and zero-point Energies= -1592.359533

Sum of electronic and thermal Energies= -1592.327770

Sum of electronic and thermal Enthalpies= -1592.326826

Sum of electronic and thermal Free Energies= -1592.419836

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	0.014535	-0.279860	0.020030
2	7	0	1.577592	1.383107	-1.648048
3	6	0	2.125081	2.574521	-0.933064
4	6	0	2.541594	2.317425	0.516186
5	6	0	0.592625	2.825628	1.929094
6	6	0	-0.714417	2.262857	2.476662
7	7	0	-1.558229	1.596806	1.437537
8	6	0	-2.142468	2.633737	0.533941
9	6	0	-2.553885	2.141804	-0.856280
10	6	0	-0.607361	2.444434	-2.340012
11	6	0	0.715394	1.826726	-2.784116
12	6	0	2.678112	0.547519	-2.206474
13	6	0	-2.623654	0.840468	2.151932
14	8	0	0.575957	-2.713020	-0.318999
15	1	0	1.348324	3.342266	-0.933439

16	1	0	2.979223	2.986702	-1.490925
17	1	0	3.375468	1.619165	0.571587
18	1	0	2.891688	3.269737	0.939464
19	1	0	0.410185	3.599614	1.178930
20	1	0	1.129991	3.313070	2.754780
21	1	0	-0.482977	1.508942	3.236152
22	1	0	-1.278048	3.066937	2.973642
23	1	0	-1.387212	3.412007	0.409174
24	1	0	-3.008962	3.108647	1.018354
25	1	0	-3.379798	1.434044	-0.800666
26	1	0	-2.916362	3.011946	-1.421882
27	1	0	-0.442920	3.328731	-1.719313
28	1	0	-1.144597	2.787010	-3.234941
29	1	0	0.503100	0.940770	-3.392381
30	1	0	1.252472	2.543994	-3.422843
31	1	0	2.226138	-0.155063	-2.917086
32	1	0	3.389044	1.166435	-2.772615
33	1	0	-2.131633	0.235044	2.922816
34	1	0	-3.309233	1.528792	2.667328
35	1	0	-0.131632	-2.639701	-1.009488
36	1	0	0.098633	-3.211225	0.368962
37	6	0	3.412382	-0.255780	-1.153301
38	6	0	4.771615	-0.568330	-1.264966
39	6	0	5.366540	-1.347184	-0.269356
40	1	0	5.348608	-0.202822	-2.108129
41	6	0	3.252753	-1.404481	0.864845
42	6	0	4.598089	-1.771175	0.816225
43	1	0	6.419518	-1.603709	-0.333321
44	1	0	5.012816	-2.360573	1.625640
45	6	0	-3.406566	-0.084832	1.247480
46	6	0	-4.781906	-0.282238	1.406641
47	6	0	-3.344047	-1.550613	-0.555210
48	6	0	-5.440660	-1.167485	0.550115
49	1	0	-5.322548	0.254737	2.179008
50	6	0	-4.712504	-1.808916	-0.451933
51	1	0	-6.507896	-1.337038	0.653163

52	1	0	-5.172590	-2.487705	-1.160165
53	7	0	-2.703363	-0.720127	0.290868
54	7	0	2.676310	-0.678344	-0.111563
55	6	0	2.368240	-1.769736	2.049345
56	8	0	1.197594	-1.221412	2.042409
57	8	0	2.827513	-2.525576	2.918970
58	6	0	-2.515812	-2.172107	-1.668900
59	8	0	-3.057936	-2.986588	-2.426865
60	8	0	-1.282428	-1.767821	-1.726315
61	7	0	-1.425617	1.484212	-1.562399
62	7	0	1.414163	1.766006	1.305293
63	1	0	1.795538	1.180690	2.051128
64	1	0	-1.819318	0.810875	-2.223173

E(RTPSSh) = -1592.88250106

Zero-point correction= 0.528700 (Hartree/Particle)

Thermal correction to Energy= 0.560140

Thermal correction to Enthalpy= 0.561084

Thermal correction to Gibbs Free Energy= 0.469000

Sum of electronic and zero-point Energies= -1592.360595

Sum of electronic and thermal Energies= -1592.329155

Sum of electronic and thermal Enthalpies= -1592.328211

Sum of electronic and thermal Free Energies= -1592.420295

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-0.008577	-0.226075	0.043722
2	7	0	-1.686738	0.970695	-1.824098
3	6	0	-0.809291	1.302122	-2.980203
4	6	0	0.349170	2.236406	-2.629094
5	6	0	1.770984	2.853219	-0.713990
6	6	0	2.461076	2.394142	0.572712
7	7	0	1.678108	1.475337	1.456793

8	6	0	0.804718	2.181222	2.434834
9	6	0	-0.323975	2.980994	1.786704
10	6	0	-1.741436	2.978839	-0.224494
11	6	0	-2.451254	2.139487	-1.288502
12	6	0	-2.671873	-0.064282	-2.251982
13	6	0	2.651028	0.639879	2.217044
14	1	0	-1.392364	1.758956	-3.794925
15	1	0	-0.406956	0.353463	-3.352142
16	1	0	0.989245	3.581988	-0.501567
17	1	0	2.524897	3.374106	-1.321104
18	1	0	3.372437	1.860257	0.292162
19	1	0	2.774922	3.282876	1.139487
20	1	0	1.398182	2.858793	3.068421
21	1	0	0.373273	1.409843	3.081140
22	1	0	-0.951856	3.587132	-0.666170
23	1	0	-2.480505	3.680840	0.187697
24	1	0	-3.367221	1.740230	-0.845563
25	1	0	-2.756842	2.798538	-2.114233
26	1	0	-3.399266	0.346216	-2.966589
27	1	0	-2.120258	-0.859422	-2.767855
28	1	0	3.366070	1.265317	2.770136
29	1	0	2.088027	0.057327	2.956240
30	6	0	-3.383226	-0.649675	-1.046952
31	6	0	-4.699189	-1.120342	-1.086656
32	6	0	-5.254143	-1.657606	0.078285
33	1	0	-5.274725	-1.060838	-2.004577
34	6	0	-3.186708	-1.205429	1.207885
35	6	0	-4.491191	-1.699545	1.247263
36	1	0	-6.274552	-2.028121	0.073735
37	1	0	-4.879990	-2.097377	2.177349
38	6	0	3.386559	-0.302908	1.285420
39	6	0	4.709065	-0.704874	1.497352
40	6	0	3.258647	-1.550759	-0.675491
41	6	0	5.305448	-1.568545	0.574752
42	1	0	5.258918	-0.341409	2.359263
43	6	0	4.575808	-1.990889	-0.537708

44	1	0	6.331587	-1.893234	0.716146
45	1	0	4.997010	-2.643140	-1.293698
46	7	0	2.681348	-0.731839	0.223643
47	7	0	-2.655477	-0.697645	0.081669
48	6	0	-2.278954	-1.206413	2.431849
49	8	0	-1.096798	-0.712854	2.234919
50	8	0	-2.720447	-1.661446	3.496087
51	6	0	2.397026	-1.965381	-1.858289
52	8	0	2.909072	-2.641571	-2.759066
53	8	0	1.162488	-1.563113	-1.803094
54	1	0	-0.956122	3.391240	2.583588
55	1	0	0.078380	3.836908	1.240705
56	1	0	-0.026097	3.232747	-2.387679
57	1	0	0.979944	2.349768	-3.518800
58	7	0	-1.122603	2.155412	0.838292
59	7	0	1.144127	1.741827	-1.468281
60	1	0	-1.873711	1.712645	1.374393
61	1	0	1.895621	1.155103	-1.840488
62	8	0	-0.535380	-2.907949	-0.180762
63	1	0	0.091375	-2.942962	-0.939081
64	1	0	-0.163091	-3.500536	0.496601

E(RTPSSh) = -1592.88590909

Zero-point correction= 0.528835 (Hartree/Particle)

Thermal correction to Energy= 0.560458

Thermal correction to Enthalpy= 0.561403

Thermal correction to Gibbs Free Energy= 0.468724

Sum of electronic and zero-point Energies= -1592.357074

Sum of electronic and thermal Energies= -1592.325451

Sum of electronic and thermal Enthalpies= -1592.324507

Sum of electronic and thermal Free Energies= -1592.417185

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-1.707554	1.880682	-0.976535
2	6	0	-0.975895	2.800259	-1.903985
3	6	0	0.094664	2.114707	-2.756964
4	6	0	2.239065	2.206589	-1.403200
5	6	0	1.952030	2.847768	-0.036670
6	7	0	1.480438	1.927912	1.045571
7	6	0	0.659992	2.696313	2.033274
8	6	0	-0.321136	1.817761	2.810510
9	6	0	-2.450427	1.887317	1.486147
10	6	0	-2.244742	2.665988	0.178008
11	6	0	-2.821172	1.233484	-1.730662
12	6	0	2.628409	1.348359	1.802432
13	1	0	-0.507108	3.576751	-1.296001
14	1	0	-1.680820	3.315651	-2.574758
15	1	0	3.101586	1.541318	-1.330221
16	1	0	2.516894	3.023054	-2.087908
17	1	0	2.862586	3.377610	0.284127
18	1	0	1.182651	3.612641	-0.162194
19	1	0	0.102329	3.459443	1.487573
20	1	0	1.308733	3.232531	2.743121
21	1	0	-3.281207	1.188268	1.385492
22	1	0	-2.741027	2.619598	2.255347
23	1	0	-3.201796	3.137800	-0.095140
24	1	0	-1.544370	3.483145	0.362894
25	1	0	-3.583347	1.983466	-1.995119
26	1	0	-2.399248	0.852631	-2.666798
27	1	0	3.311829	2.151645	2.119508
28	1	0	2.220295	0.904143	2.718640
29	6	0	-3.468743	0.083598	-0.981806
30	6	0	-4.831608	-0.208809	-1.072625
31	6	0	-5.332591	-1.310764	-0.367020
32	1	0	-5.488407	0.409829	-1.676786
33	6	0	-3.125685	-1.701730	0.487244
34	6	0	-4.473665	-2.065751	0.431959
35	1	0	-6.387686	-1.560104	-0.429727

36	1	0	-4.808003	-2.911843	1.021986
37	6	0	3.400263	0.275432	1.069953
38	6	0	4.774677	0.107160	1.256448
39	6	0	3.313254	-1.536294	-0.381356
40	6	0	5.417808	-0.953792	0.611475
41	1	0	5.327579	0.788212	1.896359
42	6	0	4.677824	-1.786723	-0.226324
43	1	0	6.482916	-1.112525	0.750364
44	1	0	5.117323	-2.610503	-0.777390
45	7	0	2.682368	-0.539278	0.275366
46	7	0	-2.643309	-0.665878	-0.226717
47	6	0	-2.131882	-2.416587	1.408660
48	8	0	-0.931048	-1.898436	1.379352
49	8	0	-2.538065	-3.346839	2.091080
50	6	0	2.485418	-2.337592	-1.373608
51	8	0	3.012819	-3.233523	-2.015254
52	8	0	1.246163	-1.917986	-1.459717
53	1	0	-0.848319	2.452216	3.539561
54	1	0	0.214909	1.054695	3.385461
55	1	0	-0.363636	1.364134	-3.407043
56	1	0	0.548525	2.880601	-3.404729
57	7	0	-1.264448	1.110849	1.919495
58	7	0	1.122747	1.402803	-1.959353
59	1	0	-1.596626	0.280308	2.411759
60	1	0	1.541554	0.706179	-2.577771
61	57	0	-0.013640	-0.276520	-0.124988
62	8	0	0.245628	-2.573434	-0.323401
63	1	0	-0.526828	-3.140222	-0.383923
64	1	0	1.125367	-2.957092	-0.344980

E(RTPSSh) = -1592.65789541

Zero-point correction= 0.529725 (Hartree/Particle)

Thermal correction to Energy= 0.560743

Thermal correction to Enthalpy= 0.561688

Thermal correction to Gibbs Free Energy= 0.470835

Sum of electronic and zero-point Energies= -1592.349326

Sum of electronic and thermal Energies= -1592.318307

Sum of electronic and thermal Enthalpies= -1592.317363

Sum of electronic and thermal Free Energies= -1592.408215

[Nd(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.918688	1.639250	1.173293
2	6	0	1.281983	2.584886	2.133740
3	6	0	-0.029298	2.049521	2.706088
4	6	0	-1.684580	2.891136	1.025079
5	6	0	-2.623193	2.406539	-0.080655
6	7	0	-1.907369	1.664420	-1.159812
7	6	0	-1.279092	2.631333	-2.105092
8	6	0	0.039643	2.122635	-2.686230
9	6	0	1.703563	2.920242	-0.986234
10	6	0	2.636976	2.401453	0.109994
11	6	0	2.873738	0.741661	1.883621
12	6	0	-2.860828	0.767514	-1.873265
13	8	0	-0.134095	-2.706065	-0.187528
14	1	0	1.089630	3.521262	1.601060
15	1	0	1.972610	2.830521	2.953604
16	1	0	0.135806	1.113441	3.248988
17	1	0	-0.432838	2.782073	3.421394
18	1	0	-0.932127	3.577255	0.621942
19	1	0	-2.270707	3.457850	1.764792
20	1	0	-3.360623	1.731108	0.361651
21	1	0	-3.176363	3.259636	-0.501280
22	1	0	-1.096393	3.560005	-1.555578
23	1	0	-1.972023	2.883906	-2.920821
24	1	0	-0.116510	1.201793	-3.257449

25	1	0	0.438176	2.877758	-3.380657
26	1	0	0.957918	3.606581	-0.570612
27	1	0	2.298284	3.497046	-1.711348
28	1	0	3.368039	1.729518	-0.348516
29	1	0	3.197883	3.240344	0.548993
30	1	0	3.715954	1.312309	2.305141
31	1	0	2.338792	0.283687	2.725433
32	1	0	-3.705831	1.336879	-2.290705
33	1	0	-2.326312	0.315309	-2.718762
34	1	0	0.189342	-3.213541	-0.961846
35	1	0	-0.190782	-3.316602	0.569197
36	6	0	3.391271	-0.341369	0.952926
37	6	0	4.663204	-0.910457	1.042266
38	6	0	5.019747	-1.900883	0.118362
39	1	0	5.359427	-0.590560	1.811325
40	6	0	2.881568	-1.637074	-0.926833
41	6	0	4.119433	-2.279525	-0.880547
42	1	0	6.000360	-2.363876	0.175044
43	1	0	4.351985	-3.042744	-1.614619
44	6	0	-3.372667	-0.319891	-0.942328
45	6	0	-4.642323	-0.893235	-1.033683
46	6	0	-2.859917	-1.609305	0.941184
47	6	0	-5.000716	-1.875804	-0.102273
48	1	0	-5.336049	-0.580461	-1.807968
49	6	0	-4.103959	-2.240805	0.904325
50	1	0	-5.980877	-2.340010	-0.157444
51	1	0	-4.337906	-2.987844	1.654368
52	7	0	-2.512789	-0.688973	0.022683
53	7	0	2.533082	-0.712559	-0.012141
54	6	0	1.791185	-1.945838	-1.949771
55	8	0	0.911870	-0.994748	-2.082150
56	8	0	1.775897	-3.060395	-2.475970
57	6	0	-1.800423	-1.919101	2.000708
58	8	0	-1.960859	-2.898823	2.721598
59	8	0	-0.789445	-1.088310	1.996606
60	7	0	-0.993546	1.740176	1.628237

61	7	0	1.003517	1.790292	-1.615487
62	1	0	-1.685958	1.096419	2.018800
63	1	0	1.687256	1.141818	-2.015265
64	60	0	0.003832	-0.097070	-0.025251

E(RTPSSh) = -1594.78643106

Zero-point correction= 0.528294 (Hartree/Particle)

Thermal correction to Energy= 0.559980

Thermal correction to Enthalpy= 0.560924

Thermal correction to Gibbs Free Energy= 0.468409

Sum of electronic and zero-point Energies= -1594.263272

Sum of electronic and thermal Energies= -1594.231586

Sum of electronic and thermal Enthalpies= -1594.230642

Sum of electronic and thermal Free Energies= -1594.323157

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	0.005530	-0.235187	0.026358
2	7	0	1.558150	1.315335	-1.687005
3	6	0	2.127178	2.525125	-1.019007
4	6	0	2.531376	2.317624	0.439905
5	6	0	0.595161	2.848488	1.866066
6	6	0	-0.691286	2.278484	2.451929
7	7	0	-1.541570	1.590737	1.433901
8	6	0	-2.142788	2.614982	0.521752
9	6	0	-2.542147	2.107520	-0.866231
10	6	0	-0.609487	2.382918	-2.383666
11	6	0	0.701793	1.744044	-2.833015
12	6	0	2.647869	0.441720	-2.208547
13	6	0	-2.594902	0.832904	2.163084
14	8	0	0.716582	-2.602081	-0.466205
15	1	0	1.366848	3.307655	-1.055265
16	1	0	2.990932	2.894537	-1.591136

17	1	0	3.369521	1.627327	0.524118
18	1	0	2.870941	3.284071	0.837646
19	1	0	0.389014	3.610668	1.109902
20	1	0	1.152394	3.347967	2.670914
21	1	0	-0.433822	1.535350	3.213542
22	1	0	-1.255285	3.080959	2.950491
23	1	0	-1.401959	3.405997	0.392037
24	1	0	-3.016871	3.076587	1.004353
25	1	0	-3.366023	1.397491	-0.808557
26	1	0	-2.902682	2.968864	-1.445500
27	1	0	-0.431172	3.288827	-1.798906
28	1	0	-1.168897	2.690807	-3.277621
29	1	0	0.476790	0.848902	-3.423060
30	1	0	1.243567	2.442494	-3.487506
31	1	0	2.189937	-0.276400	-2.899794
32	1	0	3.378864	1.026573	-2.784433
33	1	0	-2.098781	0.267917	2.961366
34	1	0	-3.306300	1.518708	2.645296
35	1	0	0.035124	-2.551998	-1.181423
36	1	0	0.397360	-3.286918	0.148817
37	6	0	3.345786	-0.337692	-1.112436
38	6	0	4.687723	-0.725441	-1.199370
39	6	0	5.240045	-1.473733	-0.157086
40	1	0	5.284141	-0.442117	-2.060373
41	6	0	3.122665	-1.369409	0.963961
42	6	0	4.449135	-1.799199	0.947290
43	1	0	6.278792	-1.786123	-0.201187
44	1	0	4.833145	-2.363026	1.789487
45	6	0	-3.335733	-0.139124	1.272852
46	6	0	-4.692016	-0.425122	1.458234
47	6	0	-3.228607	-1.555911	-0.568016
48	6	0	-5.313986	-1.333512	0.599451
49	1	0	-5.246830	0.064390	2.251849
50	6	0	-4.574804	-1.900935	-0.439351
51	1	0	-6.365217	-1.572817	0.725248
52	1	0	-5.013935	-2.584118	-1.156576

53	7	0	-2.617158	-0.714792	0.290462
54	7	0	2.589719	-0.667049	-0.053401
55	6	0	2.202069	-1.642054	2.147018
56	8	0	1.045053	-1.056784	2.083120
57	8	0	2.612001	-2.362170	3.066948
58	6	0	-2.393165	-2.069193	-1.728414
59	8	0	-2.900977	-2.867843	-2.523444
60	8	0	-1.181786	-1.592531	-1.784098
61	7	0	-1.402999	1.448228	-1.553530
62	7	0	1.399561	1.782816	1.234418
63	1	0	1.775757	1.190850	1.977330
64	1	0	-1.775329	0.727256	-2.175452

E(RTPSSh) = -1594.78797681

Zero-point correction= 0.529153 (Hartree/Particle)

Thermal correction to Energy= 0.560468

Thermal correction to Enthalpy= 0.561413

Thermal correction to Gibbs Free Energy= 0.469955

Sum of electronic and zero-point Energies= -1594.262685

Sum of electronic and thermal Energies= -1594.231370

Sum of electronic and thermal Enthalpies= -1594.230425

Sum of electronic and thermal Free Energies= -1594.321882

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	0.003379	-0.128734	-0.000103
2	7	0	-1.653858	1.196343	-1.662328
3	6	0	-0.802379	1.755751	-2.750594
4	6	0	0.324448	2.654679	-2.241754
5	6	0	1.780920	2.951236	-0.268712
6	6	0	2.458015	2.266522	0.921865
7	7	0	1.642580	1.238715	1.644609
8	6	0	0.784666	1.804623	2.724108

9	6	0	-0.350856	2.683651	2.201330
10	6	0	-1.805925	2.934612	0.223310
11	6	0	-2.479096	2.227007	-0.955353
12	6	0	-2.580182	0.185302	-2.251188
13	6	0	2.579756	0.247607	2.249260
14	8	0	0.107635	-2.646461	-0.024250
15	1	0	-1.414676	2.321692	-3.469163
16	1	0	-0.367353	0.900283	-3.275885
17	1	0	1.018080	3.657040	0.060703
18	1	0	2.548691	3.541890	-0.788602
19	1	0	3.350863	1.756493	0.551044
20	1	0	2.799620	3.037406	1.627369
21	1	0	1.389931	2.387143	3.435382
22	1	0	0.358177	0.952072	3.261263
23	1	0	-1.044195	3.635231	-0.118572
24	1	0	-2.575230	3.532923	0.731905
25	1	0	-3.367812	1.715441	-0.576558
26	1	0	-2.827325	2.984213	-1.672345
27	1	0	-3.329998	0.658778	-2.900035
28	1	0	-1.982672	-0.488228	-2.877064
29	1	0	3.326959	0.740292	2.886896
30	1	0	1.990683	-0.419059	2.890349
31	1	0	-0.325791	-3.178435	0.665933
32	1	0	-0.044637	-3.114972	-0.863962
33	6	0	-3.257902	-0.613486	-1.153524
34	6	0	-4.552775	-1.130743	-1.254191
35	6	0	-5.075699	-1.843667	-0.170918
36	1	0	-5.139713	-0.970310	-2.152459
37	6	0	-3.026914	-1.454958	1.012529
38	6	0	-4.309458	-2.003198	0.986314
39	1	0	-6.079408	-2.253632	-0.224900
40	1	0	-4.681427	-2.527602	1.858725
41	6	0	3.260809	-0.568726	1.166894
42	6	0	4.547270	-1.102376	1.289202
43	6	0	3.034095	-1.450287	-0.982891
44	6	0	5.067760	-1.844389	0.224663

45	1	0	5.128365	-0.934507	2.189958
46	6	0	4.307144	-2.018379	-0.934369
47	1	0	6.064585	-2.268524	0.295208
48	1	0	4.676218	-2.570274	-1.790953
49	7	0	2.532433	-0.755542	0.053616
50	7	0	-2.521210	-0.792405	-0.043554
51	6	0	-2.119085	-1.539446	2.235243
52	8	0	-0.964927	-0.965116	2.094911
53	8	0	-2.536844	-2.124430	3.243468
54	6	0	2.130520	-1.554516	-2.206111
55	8	0	2.535513	-2.188949	-3.189623
56	8	0	0.993623	-0.940325	-2.095847
57	1	0	-0.981508	2.975665	3.049984
58	1	0	0.042754	3.608684	1.775685
59	1	0	-0.077879	3.584225	-1.834202
60	1	0	0.953889	2.936319	-3.094928
61	7	0	-1.148033	1.989048	1.152572
62	7	0	1.125327	1.986651	-1.179114
63	1	0	-1.874408	1.449418	1.630099
64	1	0	1.851011	1.436029	-1.645244

E(RTPSSh) = -1594.79316668

Zero-point correction= 0.528549 (Hartree/Particle)

Thermal correction to Energy= 0.560408

Thermal correction to Enthalpy= 0.561352

Thermal correction to Gibbs Free Energy= 0.468856

Sum of electronic and zero-point Energies= -1594.265211

Sum of electronic and thermal Energies= -1594.233352

Sum of electronic and thermal Enthalpies= -1594.232408

Sum of electronic and thermal Free Energies= -1594.324904

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.514336	1.754511	1.186582
2	6	0	0.754201	2.422135	2.294815
3	6	0	-0.300139	1.512982	2.918104
4	6	0	-2.322202	1.964024	1.479231
5	6	0	-1.973910	2.752064	0.209278
6	7	0	-1.536051	1.936515	-0.961371
7	6	0	-0.762064	2.791843	-1.914959
8	6	0	0.267020	1.978838	-2.688822
9	6	0	2.261909	2.229413	-1.213303
10	6	0	1.903174	2.779048	0.170332
11	6	0	2.731708	1.134870	1.782643
12	6	0	-2.695992	1.420366	-1.737319
13	1	0	0.273442	3.314803	1.891718
14	1	0	1.442494	2.769475	3.076771
15	1	0	-3.238111	1.390949	1.328859
16	1	0	-2.530411	2.698528	2.270198
17	1	0	-2.843647	3.372655	-0.056108
18	1	0	-1.158804	3.442226	0.433043
19	1	0	-0.261271	3.581634	-1.353913
20	1	0	-1.438185	3.297043	-2.618834
21	1	0	3.205250	1.684372	-1.176692
22	1	0	2.418849	3.091296	-1.877118
23	1	0	2.749278	3.378141	0.539361
24	1	0	1.058287	3.460587	0.073255
25	1	0	3.434831	1.915954	2.105765
26	1	0	2.416721	0.598523	2.685986
27	1	0	-3.386697	2.243661	-1.972568
28	1	0	-2.307244	1.048382	-2.692419
29	6	0	3.429620	0.150827	0.869551
30	6	0	4.807994	-0.080436	0.941787
31	6	0	5.369689	-1.057915	0.117793
32	1	0	5.422576	0.494107	1.626961
33	6	0	3.183670	-1.474679	-0.778236
34	6	0	4.546533	-1.771044	-0.756080
35	1	0	6.436330	-1.255994	0.155796
36	1	0	4.930713	-2.539919	-1.416079

37	6	0	-3.451591	0.294724	-1.080756
38	6	0	-4.833146	0.149030	-1.257679
39	6	0	-3.359399	-1.616284	0.222943
40	6	0	-5.476755	-0.946468	-0.681706
41	1	0	-5.386548	0.883687	-1.833394
42	6	0	-4.726515	-1.847616	0.074632
43	1	0	-6.546161	-1.083544	-0.807837
44	1	0	-5.170592	-2.706588	0.563925
45	7	0	-2.728075	-0.575898	-0.358625
46	7	0	2.646547	-0.531894	0.019245
47	6	0	2.218308	-2.200769	-1.704105
48	8	0	0.994196	-1.772408	-1.656150
49	8	0	2.651387	-3.112506	-2.419976
50	6	0	-2.505959	-2.500714	1.105266
51	8	0	-2.984468	-3.532815	1.589064
52	8	0	-1.307583	-2.041042	1.293654
53	1	0	0.779899	2.639756	-3.402324
54	1	0	-0.220746	1.187806	-3.268195
55	1	0	0.174553	0.636820	3.373870
56	1	0	-0.804498	2.067126	3.722817
57	7	0	1.228798	1.320996	-1.775270
58	7	0	-1.271166	1.006984	1.919340
59	1	0	1.714292	0.609338	-2.321849
60	1	0	-1.750438	0.216276	2.352449
61	60	0	0.021382	-0.321924	0.012912
62	8	0	1.152368	-2.222065	1.583658
63	1	0	1.633673	-2.033372	2.407713
64	1	0	0.244390	-2.525512	1.842353

E(RTPSSh) = -1594.77976106

Zero-point correction= 0.529644 (Hartree/Particle)

Thermal correction to Energy= 0.560850

Thermal correction to Enthalpy= 0.561795

Thermal correction to Gibbs Free Energy= 0.470197

Sum of electronic and zero-point Energies= -1594.250117

Sum of electronic and thermal Energies= -1594.218911

Sum of electronic and thermal Enthalpies= -1594.217966

Sum of electronic and thermal Free Energies= -1594.309564

[Eu(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.003927	-0.066781	-0.019843
2	7	0	1.871412	1.617975	1.210673
3	6	0	1.222650	2.558085	2.168624
4	6	0	-0.109223	2.030733	2.696691
5	6	0	-1.714755	2.878631	0.966536
6	6	0	-2.622584	2.383323	-0.159728
7	7	0	-1.871013	1.627825	-1.204984
8	6	0	-1.232539	2.586327	-2.152062
9	6	0	0.107747	2.084143	-2.684685
10	6	0	1.716693	2.908222	-0.941124
11	6	0	2.622415	2.391327	0.178321
12	6	0	2.796132	0.691081	1.923440
13	6	0	-2.792013	0.698471	-1.919760
14	8	0	-0.080380	-2.660903	-0.114154
15	1	0	1.055209	3.503146	1.642726
16	1	0	1.894789	2.783929	3.009092
17	1	0	0.031590	1.091931	3.240783
18	1	0	-0.533807	2.765023	3.397614
19	1	0	-0.956063	3.567760	0.580613
20	1	0	-2.320641	3.442495	1.692202
21	1	0	-3.374243	1.714275	0.268658
22	1	0	-3.162227	3.230086	-0.608965
23	1	0	-1.077499	3.526951	-1.614404
24	1	0	-1.906622	2.813531	-2.990531
25	1	0	-0.021049	1.154837	-3.247950

26	1	0	0.525232	2.835864	-3.371307
27	1	0	0.960624	3.595418	-0.546325
28	1	0	2.326700	3.480832	-1.656555
29	1	0	3.372516	1.727856	-0.261770
30	1	0	3.163877	3.229318	0.641879
31	1	0	3.638246	1.237237	2.376000
32	1	0	2.234071	0.221149	2.740423
33	1	0	-3.639037	1.241081	-2.367261
34	1	0	-2.230179	0.235903	-2.741287
35	1	0	0.153382	-3.200348	-0.895067
36	1	0	-0.083028	-3.245464	0.664541
37	6	0	3.313393	-0.376073	0.974076
38	6	0	4.577689	-0.962218	1.060902
39	6	0	4.934797	-1.927397	0.110764
40	1	0	5.268122	-0.673111	1.847117
41	6	0	2.808249	-1.615644	-0.946086
42	6	0	4.042366	-2.265656	-0.909549
43	1	0	5.910474	-2.401203	0.163536
44	1	0	4.275912	-3.004921	-1.667434
45	6	0	-3.299792	-0.374018	-0.969542
46	6	0	-4.560574	-0.967510	-1.055298
47	6	0	-2.788175	-1.601106	0.957101
48	6	0	-4.915851	-1.924676	-0.096473
49	1	0	-5.250495	-0.688001	-1.845463
50	6	0	-4.025622	-2.245412	0.930964
51	1	0	-5.889735	-2.402516	-0.146216
52	1	0	-4.259616	-2.968092	1.704499
53	7	0	-2.444231	-0.705786	0.012940
54	7	0	2.461157	-0.713755	-0.008920
55	6	0	1.732975	-1.889576	-1.996470
56	8	0	0.810245	-0.968774	-2.057312
57	8	0	1.781115	-2.945203	-2.625864
58	6	0	-1.736283	-1.861543	2.036844
59	8	0	-1.913092	-2.790893	2.817370
60	8	0	-0.714289	-1.044269	1.989483
61	7	0	-1.035930	1.728007	1.583999

62	7	0	1.035341	1.770066	-1.576247
63	1	0	-1.740045	1.083105	1.949587
64	1	0	1.734045	1.122028	-1.947984

E(RTPSSh) = -1596.60321081

Zero-point correction= 0.529281 (Hartree/Particle)

Thermal correction to Energy= 0.560505

Thermal correction to Enthalpy= 0.561449

Thermal correction to Gibbs Free Energy= 0.470684

Sum of electronic and zero-point Energies= -1596.079694

Sum of electronic and thermal Energies= -1596.048471

Sum of electronic and thermal Enthalpies= -1596.047527

Sum of electronic and thermal Free Energies= -1596.138291

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000015	0.106614	-0.000028
2	7	0	-1.576885	-1.453873	-1.564037
3	6	0	-2.184141	-2.586054	-0.799917
4	6	0	-2.513912	-2.275102	0.664122
5	6	0	-0.550879	-2.667514	2.159742
6	6	0	0.728736	-1.996465	2.668742
7	7	0	1.576901	-1.453918	1.563995
8	6	0	2.184104	-2.586121	0.799870
9	6	0	2.513898	-2.275167	-0.664162
10	6	0	0.550858	-2.667535	-2.159780
11	6	0	-0.728741	-1.996457	-2.668783
12	6	0	-2.626995	-0.564863	-2.142157
13	6	0	2.627053	-0.564954	2.142109
14	8	0	-0.000087	2.672268	-0.000132
15	1	0	-1.465230	-3.408296	-0.814001
16	1	0	-3.087610	-2.946043	-1.315610
17	1	0	-3.334066	-1.560074	0.737237

18	1	0	-2.856503	-3.203901	1.141739
19	1	0	-0.331453	-3.539308	1.534644
20	1	0	-1.114097	-3.038251	3.029081
21	1	0	0.448167	-1.149886	3.304148
22	1	0	1.296061	-2.708719	3.287403
23	1	0	1.465147	-3.408323	0.813932
24	1	0	3.087548	-2.946169	1.315567
25	1	0	3.334065	-1.560153	-0.737269
26	1	0	2.856475	-3.203969	-1.141783
27	1	0	0.331406	-3.539320	-1.534677
28	1	0	1.114067	-3.038293	-3.029117
29	1	0	-0.448150	-1.149893	-3.304201
30	1	0	-1.296090	-2.708700	-3.287432
31	1	0	-2.136326	0.072242	-2.888684
32	1	0	-3.394946	-1.152512	-2.667744
33	1	0	2.136423	0.072139	2.888673
34	1	0	3.395003	-1.152639	2.667657
35	1	0	0.159346	3.243468	-0.773097
36	1	0	-0.159045	3.243497	0.772901
37	6	0	-3.267080	0.328711	-1.095000
38	6	0	-4.590966	0.770553	-1.151381
39	6	0	-5.052295	1.635153	-0.151209
40	1	0	-5.246045	0.450429	-1.955663
41	6	0	-2.898285	1.510092	0.890556
42	6	0	-4.197610	2.018948	0.884998
43	1	0	-6.075970	1.996454	-0.179044
44	1	0	-4.507381	2.684509	1.682838
45	6	0	3.267132	0.328648	1.094974
46	6	0	4.591016	0.770493	1.151364
47	6	0	2.898309	1.510152	-0.890503
48	6	0	5.052325	1.635167	0.151248
49	1	0	5.246108	0.450322	1.955618
50	6	0	4.197619	2.019042	-0.884914
51	1	0	6.075996	1.996478	0.179097
52	1	0	4.507371	2.684691	-1.682687
53	7	0	2.454737	0.703826	0.092335

54	7	0	-2.454692	0.703846	-0.092338
55	6	0	-1.884467	1.825243	1.990764
56	8	0	-0.856020	1.013678	2.008994
57	8	0	-2.090129	2.785841	2.724994
58	6	0	1.884413	1.825403	-1.990607
59	8	0	2.089801	2.786338	-2.724483
60	8	0	0.856158	1.013614	-2.009071
61	7	0	1.339334	-1.710210	-1.362920
62	7	0	-1.339334	-1.710171	1.362879
63	1	0	-1.641029	-0.955525	1.986603
64	1	0	1.641045	-0.955562	-1.986636

E(RTPSSh) = -1596.60507823

Zero-point correction= 0.529806 (Hartree/Particle)

Thermal correction to Energy= 0.561187

Thermal correction to Enthalpy= 0.562131

Thermal correction to Gibbs Free Energy= 0.470280

Sum of electronic and zero-point Energies= -1596.079658

Sum of electronic and thermal Energies= -1596.048278

Sum of electronic and thermal Enthalpies= -1596.047334

Sum of electronic and thermal Free Energies= -1596.139185

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	-0.000022	0.058289	-0.000048
2	7	0	1.662548	-1.231884	-1.625795
3	6	0	0.826398	-1.795162	-2.721766
4	6	0	-0.308366	-2.690526	-2.218943
5	6	0	-1.810486	-2.957828	-0.270494
6	6	0	-2.489379	-2.249038	0.908715
7	7	0	-1.662459	-1.232270	1.625544
8	6	0	-0.826258	-1.795678	2.721409
9	6	0	0.308556	-2.690879	2.218427

10	6	0	1.810666	-2.957749	0.269932
11	6	0	2.489529	-2.248728	-0.909148
12	6	0	2.573221	-0.192098	-2.192720
13	6	0	-2.573203	-0.192673	2.192704
14	8	0	0.000095	2.629688	-0.000188
15	1	0	1.445033	-2.368052	-3.431199
16	1	0	0.395697	-0.940643	-3.251287
17	1	0	-1.065712	-3.676457	0.077109
18	1	0	-2.582095	-3.540277	-0.796862
19	1	0	-3.368844	-1.725109	0.523388
20	1	0	-2.856396	-3.008238	1.616193
21	1	0	-1.444848	-2.368721	3.430757
22	1	0	-0.395606	-0.941212	3.251061
23	1	0	1.065911	-3.676335	-0.077800
24	1	0	2.582289	-3.540269	0.796200
25	1	0	3.368970	-1.724823	-0.523733
26	1	0	2.856581	-3.007786	-1.616760
27	1	0	3.344153	-0.640509	-2.837008
28	1	0	1.960213	0.469275	-2.817211
29	1	0	-3.344087	-0.641280	2.836912
30	1	0	-1.960230	0.468615	2.817319
31	1	0	0.122284	3.201565	0.777180
32	1	0	-0.122750	3.201521	-0.777491
33	6	0	3.208150	0.616595	-1.074663
34	6	0	4.477697	1.195697	-1.132243
35	6	0	4.922374	1.941642	-0.033020
36	1	0	5.103795	1.068697	-2.009991
37	6	0	2.851263	1.467880	1.075941
38	6	0	4.103484	2.084055	1.089917
39	1	0	5.905892	2.401580	-0.055237
40	1	0	4.401747	2.650586	1.964967
41	6	0	-3.208211	0.616217	1.074841
42	6	0	-4.477792	1.195230	1.132573
43	6	0	-2.851397	1.468037	-1.075562
44	6	0	-4.922515	1.941431	0.033541
45	1	0	-5.103877	1.067977	2.010293

46	6	0	-4.103632	2.084190	-1.089360
47	1	0	-5.906057	2.401313	0.055880
48	1	0	-4.401916	2.650972	-1.964241
49	7	0	-2.431518	0.759143	-0.012630
50	7	0	2.431428	0.759232	0.012827
51	6	0	1.859577	1.570756	2.235948
52	8	0	0.775976	0.853794	2.071495
53	8	0	2.135226	2.300329	3.181894
54	6	0	-1.859669	1.571290	-2.235499
55	8	0	-2.135011	2.301648	-3.180935
56	8	0	-0.776340	0.853821	-2.071507
57	1	0	0.927293	-2.981358	3.077797
58	1	0	-0.085921	-3.618345	1.795644
59	1	0	0.086167	-3.618049	-1.796335
60	1	0	-0.927083	-2.980882	-3.078369
61	7	0	1.116233	-2.014038	1.169032
62	7	0	-1.116086	-2.013934	-1.169423
63	1	0	1.807352	-1.425049	1.641688
64	1	0	-1.807203	-1.424855	-1.641974

E(RTPSSh) = -1596.61087656

Zero-point correction= 0.528555 (Hartree/Particle)

Thermal correction to Energy= 0.560478

Thermal correction to Enthalpy= 0.561422

Thermal correction to Gibbs Free Energy= 0.468251

Sum of electronic and zero-point Energies= -1596.085065

Sum of electronic and thermal Energies= -1596.053142

Sum of electronic and thermal Enthalpies= -1596.052198

Sum of electronic and thermal Free Energies= -1596.145369

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.524864	-1.898288	-1.028165

2	6	0	0.778164	-2.659464	-2.078839
3	6	0	-0.185261	-1.756042	-2.836336
4	6	0	-2.273514	-2.020208	-1.494494
5	6	0	-2.006937	-2.721805	-0.160319
6	7	0	-1.604033	-1.818743	0.962158
7	6	0	-0.918825	-2.631021	2.024121
8	6	0	0.146297	-1.848581	2.789713
9	6	0	2.237262	-2.125845	1.409297
10	6	0	1.902027	-2.817704	0.086579
11	6	0	2.738387	-1.356695	-1.700951
12	6	0	-2.814499	-1.192659	1.567557
13	1	0	0.229616	-3.471496	-1.600893
14	1	0	1.475543	-3.132107	-2.783898
15	1	0	-3.184864	-1.423452	-1.440937
16	1	0	-2.448089	-2.800018	-2.248568
17	1	0	-2.900499	-3.299146	0.119378
18	1	0	-1.200505	-3.443449	-0.290259
19	1	0	-0.465625	-3.500914	1.546328
20	1	0	-1.654305	-3.022887	2.739339
21	1	0	3.143021	-1.525709	1.306527
22	1	0	2.450314	-2.909524	2.149441
23	1	0	2.758138	-3.444314	-0.204919
24	1	0	1.059417	-3.492966	0.241022
25	1	0	3.451380	-2.169784	-1.898596
26	1	0	2.424075	-0.967652	-2.676307
27	1	0	-3.579419	-1.958983	1.757062
28	1	0	-2.523322	-0.789121	2.542069
29	6	0	3.425798	-0.228068	-0.975952
30	6	0	4.804231	-0.017199	-1.103323
31	6	0	5.374403	1.105708	-0.503031
32	1	0	5.410582	-0.719166	-1.666233
33	6	0	3.196235	1.683859	0.315072
34	6	0	4.554928	1.977923	0.215342
35	1	0	6.439891	1.292994	-0.591568
36	1	0	4.938121	2.866076	0.703782
37	6	0	-3.399726	-0.067763	0.741895

38	6	0	-4.762341	0.246986	0.774550
39	6	0	-2.971623	1.695159	-0.719348
40	6	0	-5.219775	1.339769	0.034089
41	1	0	-5.446725	-0.353117	1.365099
42	6	0	-4.312232	2.079912	-0.726256
43	1	0	-6.272813	1.603003	0.045880
44	1	0	-4.614940	2.932337	-1.322989
45	7	0	-2.534518	0.646981	0.003513
46	7	0	2.641280	0.602610	-0.270551
47	6	0	2.255184	2.558088	1.115389
48	8	0	1.049216	2.085774	1.199104
49	8	0	2.673304	3.602951	1.625340
50	6	0	-1.911750	2.422779	-1.533296
51	8	0	-2.243043	3.407489	-2.204374
52	8	0	-0.722210	1.910779	-1.443842
53	1	0	0.620265	-2.528415	3.511406
54	1	0	-0.314210	-1.033837	3.351863
55	1	0	0.356824	-0.945571	-3.334411
56	1	0	-0.690756	-2.342196	-3.616471
57	7	0	1.161882	-1.221510	1.901242
58	7	0	-1.163744	-1.124095	-1.918381
59	63	0	-0.007695	0.210546	0.059094
60	1	0	1.624196	-0.505387	2.464472
61	1	0	-1.582518	-0.345221	-2.427059
62	8	0	-0.926332	1.109949	2.323609
63	1	0	-0.237677	1.817175	2.385024
64	1	0	-1.426541	1.101450	3.155320

E(RTPSSh) = -1596.60008192

Zero-point correction= 0.530688 (Hartree/Particle)

Thermal correction to Energy= 0.561608

Thermal correction to Enthalpy= 0.562552

Thermal correction to Gibbs Free Energy= 0.471262

Sum of electronic and zero-point Energies= -1596.074577

Sum of electronic and thermal Energies= -1596.043657

Sum of electronic and thermal Enthalpies= -1596.042713

Sum of electronic and thermal Free Energies= -1596.134003

[Gd(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.003599	-0.059404	-0.016972
2	7	0	1.853257	1.611708	1.224791
3	6	0	1.199318	2.551017	2.180040
4	6	0	-0.139654	2.027612	2.693285
5	6	0	-1.727823	2.874269	0.945247
6	6	0	-2.623380	2.374318	-0.188778
7	7	0	-1.858583	1.614662	-1.221365
8	6	0	-1.215640	2.570303	-2.168274
9	6	0	0.131666	2.070899	-2.684729
10	6	0	1.720751	2.902789	-0.925834
11	6	0	2.615819	2.387471	0.202726
12	6	0	2.767249	0.675941	1.939951
13	6	0	-2.767516	0.674234	-1.937285
14	8	0	-0.060072	-2.651630	-0.087941
15	1	0	1.040618	3.498193	1.655203
16	1	0	1.864365	2.771398	3.027518
17	1	0	-0.007460	1.089225	3.239976
18	1	0	-0.571253	2.764211	3.387361
19	1	0	-0.966965	3.564599	0.565787
20	1	0	-2.341669	3.437333	1.664756
21	1	0	-3.379781	1.706950	0.234056
22	1	0	-3.158297	3.218454	-0.648263
23	1	0	-1.069885	3.514559	-1.634394
24	1	0	-1.882677	2.789491	-3.014433
25	1	0	0.012068	1.139555	-3.246342
26	1	0	0.555313	2.822465	-3.367606

27	1	0	0.960215	3.589626	-0.539160
28	1	0	2.336502	3.474454	-1.636980
29	1	0	3.372565	1.726295	-0.229495
30	1	0	3.150146	3.225705	0.673790
31	1	0	3.607912	1.214572	2.403966
32	1	0	2.195164	0.202193	2.747692
33	1	0	-3.613724	1.207599	-2.397174
34	1	0	-2.194854	0.207307	-2.748742
35	1	0	0.134882	-3.202178	-0.870204
36	1	0	-0.056943	-3.229768	0.695431
37	6	0	3.287203	-0.385767	0.985684
38	6	0	4.549354	-0.976265	1.074082
39	6	0	4.910036	-1.931673	0.115419
40	1	0	5.235714	-0.697207	1.867449
41	6	0	2.789242	-1.605928	-0.949401
42	6	0	4.023338	-2.256043	-0.914382
43	1	0	5.884497	-2.407948	0.168595
44	1	0	4.260316	-2.985069	-1.681064
45	6	0	-3.276679	-0.392101	-0.980873
46	6	0	-4.535340	-0.990288	-1.065291
47	6	0	-2.768691	-1.598783	0.960244
48	6	0	-4.891682	-1.938249	-0.097647
49	1	0	-5.223069	-0.720937	-1.860857
50	6	0	-4.004790	-2.245699	0.936798
51	1	0	-5.864177	-2.419057	-0.145989
52	1	0	-4.240373	-2.960101	1.717513
53	7	0	-2.423996	-0.712446	0.007921
54	7	0	2.439373	-0.713088	-0.004730
55	6	0	1.724226	-1.867010	-2.014289
56	8	0	0.778145	-0.967095	-2.045711
57	8	0	1.807057	-2.890362	-2.689799
58	6	0	-1.719755	-1.844687	2.046324
59	8	0	-1.900909	-2.760842	2.841336
60	8	0	-0.695568	-1.030733	1.989312
61	7	0	-1.053190	1.724780	1.569476
62	7	0	1.047011	1.761746	-1.564356

63	1	0	-1.761130	1.079849	1.927278
64	1	0	1.751819	1.115682	-1.927318

E(RTPSSh) = -1597.19246050

Zero-point correction= 0.529459 (Hartree/Particle)

Thermal correction to Energy= 0.560615

Thermal correction to Enthalpy= 0.561559

Thermal correction to Gibbs Free Energy= 0.471032

Sum of electronic and zero-point Energies= -1596.669774

Sum of electronic and thermal Energies= -1596.638618

Sum of electronic and thermal Enthalpies= -1596.637674

Sum of electronic and thermal Free Energies= -1596.728202

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.564793	1.444719	1.571264
2	6	0	-2.183445	2.576910	0.816322
3	6	0	-2.517459	2.270866	-0.647718
4	6	0	-0.561280	2.663655	-2.153729
5	6	0	0.712087	1.987988	-2.672143
6	7	0	1.564736	1.444557	-1.571447
7	6	0	2.183447	2.576739	-0.816542
8	6	0	2.517465	2.270738	0.647505
9	6	0	0.561307	2.663685	2.153461
10	6	0	-0.712094	1.988138	2.671924
11	6	0	-2.605809	0.546679	2.151683
12	6	0	2.605699	0.546399	-2.151783
13	8	0	0.000764	-2.657066	-0.000587
14	1	0	-1.470089	3.403882	0.831731
15	1	0	-3.086925	2.927748	1.338094
16	1	0	-3.338307	1.556514	-0.720593
17	1	0	-2.860727	3.201031	-1.121997
18	1	0	-0.334643	3.534617	-1.530056

19	1	0	-1.130883	3.035557	-3.018331
20	1	0	0.424055	1.141272	-3.303875
21	1	0	1.277995	2.697421	-3.295207
22	1	0	1.470131	3.403744	-0.831983
23	1	0	3.086943	2.927511	-1.338331
24	1	0	3.338303	1.556382	0.720406
25	1	0	2.860736	3.200917	1.121752
26	1	0	0.334730	3.534601	1.529703
27	1	0	1.130934	3.035633	3.018028
28	1	0	-0.424108	1.141431	3.303691
29	1	0	-1.277941	2.697641	3.294964
30	1	0	-2.106273	-0.092134	2.890770
31	1	0	-3.373974	1.126749	2.685213
32	1	0	2.106124	-0.092472	-2.890795
33	1	0	3.373884	1.126377	-2.685386
34	1	0	0.139911	-3.228335	0.775803
35	1	0	-0.142399	-3.228475	-0.776179
36	6	0	-3.246171	-0.343422	1.101786
37	6	0	-4.567792	-0.791985	1.158814
38	6	0	-5.028717	-1.649406	0.152285
39	1	0	-5.221569	-0.481893	1.968056
40	6	0	-2.878501	-1.506595	-0.895091
41	6	0	-4.176142	-2.019591	-0.890705
42	1	0	-6.050753	-2.015317	0.180195
43	1	0	-4.486137	-2.677770	-1.694563
44	6	0	3.246029	-0.343599	-1.101771
45	6	0	4.567605	-0.792288	-1.158814
46	6	0	2.878402	-1.506295	0.895384
47	6	0	5.028551	-1.649477	-0.152099
48	1	0	5.221336	-0.482452	-1.968193
49	6	0	4.176049	-2.019276	0.891080
50	1	0	6.050557	-2.015473	-0.179999
51	1	0	4.486080	-2.677153	1.695170
52	7	0	2.435295	-0.707412	-0.093659
53	7	0	-2.435412	-0.707485	0.093784
54	6	0	-1.867948	-1.806460	-2.002693

55	8	0	-0.833372	-1.001927	-2.005810
56	8	0	-2.082766	-2.747798	-2.758600
57	6	0	1.868127	-1.805732	2.003355
58	8	0	2.084058	-2.745595	2.760746
59	8	0	0.832643	-1.002304	2.005405
60	7	0	1.344895	1.707057	1.350671
61	7	0	-1.344905	1.707141	-1.350853
62	1	0	-1.648200	0.952530	-1.973514
63	1	0	1.648217	0.952566	1.973446
64	64	0	-0.000044	-0.098300	-0.000135

E(RTPSSh) = -1597.19475564

Zero-point correction= 0.530003 (Hartree/Particle)

Thermal correction to Energy= 0.561260

Thermal correction to Enthalpy= 0.562204

Thermal correction to Gibbs Free Energy= 0.470879

Sum of electronic and zero-point Energies= -1596.669669

Sum of electronic and thermal Energies= -1596.638412

Sum of electronic and thermal Enthalpies= -1596.637467

Sum of electronic and thermal Free Energies= -1596.728793

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.048515	0.000000
2	7	0	-1.657361	-1.227385	1.625508
3	6	0	-0.823553	-1.793185	2.721765
4	6	0	0.310698	-2.687718	2.216803
5	6	0	1.812661	-2.952713	0.268523
6	6	0	2.488659	-2.242393	-0.911181
7	7	0	1.657360	-1.227380	-1.625511
8	6	0	0.823552	-1.793175	-2.721771
9	6	0	-0.310700	-2.687709	-2.216812
10	6	0	-1.812662	-2.952711	-0.268532

11	6	0	-2.488661	-2.242394	0.911173
12	6	0	-2.563600	-0.183124	2.190906
13	6	0	2.563600	-0.183118	-2.190905
14	8	0	0.000006	2.611266	-0.000006
15	1	0	-1.443508	-2.367362	3.428925
16	1	0	-0.392816	-0.940015	3.253056
17	1	0	1.069718	-3.673744	-0.078189
18	1	0	2.585786	-3.532338	0.795663
19	1	0	3.367582	-1.716697	-0.527000
20	1	0	2.856119	-3.000176	-1.619849
21	1	0	1.443507	-2.367349	-3.428933
22	1	0	0.392816	-0.940002	-3.253058
23	1	0	-1.069719	-3.673742	0.078176
24	1	0	-2.585787	-3.532334	-0.795675
25	1	0	-3.367583	-1.716697	0.526994
26	1	0	-2.856121	-3.000179	1.619839
27	1	0	-3.337137	-0.627116	2.835066
28	1	0	-1.947610	0.476558	2.814078
29	1	0	3.337136	-0.627107	-2.835067
30	1	0	1.947610	0.476568	-2.814075
31	1	0	-0.110040	3.182800	-0.779332
32	1	0	0.110040	3.182807	0.779319
33	6	0	-3.193024	0.625945	1.070332
34	6	0	-4.458798	1.213693	1.124296
35	6	0	-4.897557	1.958040	0.021690
36	1	0	-5.086504	1.094260	2.001950
37	6	0	-2.828110	1.467537	-1.082711
38	6	0	-4.076519	2.090998	-1.100949
39	1	0	-5.878147	2.424313	0.041049
40	1	0	-4.370315	2.656036	-1.978476
41	6	0	3.193024	0.625947	-1.070329
42	6	0	4.458798	1.213696	-1.124291
43	6	0	2.828110	1.467532	1.082717
44	6	0	4.897557	1.958039	-0.021683
45	1	0	5.086503	1.094266	-2.001945
46	6	0	4.076519	2.090994	1.100957

47	1	0	5.878146	2.424313	-0.041039
48	1	0	4.370314	2.656029	1.978486
49	7	0	2.414223	0.759766	0.016688
50	7	0	-2.414223	0.759767	-0.016684
51	6	0	-1.832507	1.561225	-2.239655
52	8	0	-0.751625	0.841768	-2.067496
53	8	0	-2.101712	2.286634	-3.190638
54	6	0	1.832507	1.561218	2.239661
55	8	0	2.101715	2.286617	3.190650
56	8	0	0.751621	0.841767	2.067497
57	1	0	-0.931470	-2.978589	-3.074545
58	1	0	0.083859	-3.614980	-1.793659
59	1	0	-0.083862	-3.614986	1.793644
60	1	0	0.931467	-2.978603	3.074535
61	7	0	-1.115904	-2.009360	-1.166324
62	7	0	1.115904	-2.009365	1.166318
63	1	0	-1.805815	-1.418671	-1.638612
64	1	0	1.805815	-1.418679	1.638609

E(RTPSSh) = -1597.20089365

Zero-point correction= 0.529023 (Hartree/Particle)

Thermal correction to Energy= 0.560676

Thermal correction to Enthalpy= 0.561620

Thermal correction to Gibbs Free Energy= 0.469714

Sum of electronic and zero-point Energies= -1596.674955

Sum of electronic and thermal Energies= -1596.643302

Sum of electronic and thermal Enthalpies= -1596.642358

Sum of electronic and thermal Free Energies= -1596.734264

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.591763	-1.820470	0.968108
2	6	0	-0.866585	-2.633442	1.998760

3	6	0	0.163825	-1.823532	2.780974
4	6	0	2.291124	-2.020124	1.451721
5	6	0	2.000254	-2.769555	0.148809
6	7	0	1.544922	-1.901965	-0.979138
7	6	0	0.789930	-2.719542	-1.979766
8	6	0	-0.186263	-1.869811	-2.786338
9	6	0	-2.310267	-2.015681	-1.471305
10	6	0	-2.061875	-2.717395	-0.133274
11	6	0	-2.762508	-1.178934	1.628949
12	6	0	2.716489	-1.330572	-1.702438
13	1	0	-0.377212	-3.464154	1.489226
14	1	0	-1.579482	-3.081335	2.705083
15	1	0	3.166215	-1.379031	1.334913
16	1	0	2.537417	-2.766892	2.219321
17	1	0	2.900042	-3.332267	-0.139621
18	1	0	1.216664	-3.507610	0.323211
19	1	0	0.248745	-3.502204	-1.447847
20	1	0	1.482265	-3.229941	-2.663840
21	1	0	-3.189411	-1.373133	-1.411621
22	1	0	-2.530318	-2.790840	-2.218299
23	1	0	-2.983397	-3.237013	0.166974
24	1	0	-1.303449	-3.489385	-0.266165
25	1	0	-3.526734	-1.933932	1.860849
26	1	0	-2.417869	-0.768121	2.583164
27	1	0	3.434162	-2.127685	-1.942636
28	1	0	2.352622	-0.931022	-2.656067
29	6	0	-3.372444	-0.061144	0.810503
30	6	0	-4.735390	0.248458	0.860486
31	6	0	-5.208897	1.329816	0.113050
32	1	0	-5.407768	-0.347986	1.468114
33	6	0	-2.975686	1.685496	-0.685459
34	6	0	-4.318601	2.061924	-0.675098
35	1	0	-6.262704	1.588721	0.138778
36	1	0	-4.637450	2.900983	-1.282176
37	6	0	3.408053	-0.204256	-0.977427
38	6	0	4.787474	0.004436	-1.084471

39	6	0	3.161542	1.704327	0.318832
40	6	0	5.351692	1.120246	-0.463403
41	1	0	5.400293	-0.693484	-1.645199
42	6	0	4.524581	1.989339	0.249865
43	1	0	6.418942	1.304837	-0.533952
44	1	0	4.903993	2.871191	0.752448
45	7	0	2.615170	0.627675	-0.280999
46	7	0	-2.520509	0.653893	0.051786
47	6	0	-1.937491	2.392800	-1.545495
48	8	0	-0.754575	1.862988	-1.504079
49	8	0	-2.285005	3.376085	-2.210663
50	6	0	2.200823	2.590068	1.083193
51	8	0	2.623979	3.588356	1.674241
52	8	0	0.966207	2.184822	1.034269
53	1	0	-0.694066	-2.512979	-3.518123
54	1	0	0.348268	-1.097339	-3.347921
55	1	0	-0.327947	-1.029532	3.346730
56	1	0	0.658973	-2.494996	3.496053
57	7	0	-1.166785	-1.173439	-1.915124
58	7	0	1.166391	-1.156208	1.904368
59	1	0	-1.555363	-0.408256	-2.467607
60	1	0	1.583624	-0.415962	2.471406
61	64	0	-0.003099	0.192221	-0.000303
62	8	0	-0.814187	1.036987	2.347092
63	1	0	-0.157498	1.777024	2.229203
64	1	0	-1.685200	1.472320	2.361085

E(RTPSSh) = -1597.19484833

Zero-point correction= 0.530870 (Hartree/Particle)

Thermal correction to Energy= 0.561743

Thermal correction to Enthalpy= 0.562687

Thermal correction to Gibbs Free Energy= 0.471326

Sum of electronic and zero-point Energies= -1596.664234

Sum of electronic and thermal Energies= -1596.633361

Sum of electronic and thermal Enthalpies= -1596.632417

Sum of electronic and thermal Free Energies= -1596.723779

[Ho(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.001141	-0.033518	-0.005833
2	7	0	1.811805	1.586387	1.260325
3	6	0	1.151331	2.527814	2.208974
4	6	0	-0.208064	2.023181	2.683722
5	6	0	-1.749917	2.867940	0.890005
6	6	0	-2.615515	2.354995	-0.261515
7	7	0	-1.817848	1.583415	-1.259725
8	6	0	-1.162698	2.530833	-2.206316
9	6	0	0.200547	2.036669	-2.681538
10	6	0	1.741209	2.880302	-0.884412
11	6	0	2.607574	2.364073	0.265429
12	6	0	2.691814	0.620610	1.978965
13	6	0	-2.695012	0.614341	-1.977727
14	8	0	-0.017828	-2.634648	-0.024327
15	1	0	1.021320	3.481386	1.687629
16	1	0	1.799269	2.729580	3.074031
17	1	0	-0.102582	1.086983	3.238930
18	1	0	-0.654560	2.769782	3.357079
19	1	0	-0.982707	3.559244	0.525265
20	1	0	-2.381794	3.431196	1.593376
21	1	0	-3.383151	1.692191	0.148523
22	1	0	-3.138243	3.191509	-0.747564
23	1	0	-1.039136	3.484075	-1.682756
24	1	0	-1.811409	2.730247	-3.071313
25	1	0	0.101492	1.102274	-3.241001
26	1	0	0.642809	2.788771	-3.351566
27	1	0	0.972760	3.569072	-0.517442

28	1	0	2.372596	3.447341	-1.585195
29	1	0	3.376400	1.704361	-0.147483
30	1	0	3.128725	3.199574	0.754978
31	1	0	3.530766	1.132716	2.474611
32	1	0	2.089868	0.138074	2.759156
33	1	0	-3.536647	1.123155	-2.472152
34	1	0	-2.092382	0.134325	-2.758994
35	1	0	0.061295	-3.205326	-0.809946
36	1	0	-0.017110	-3.207434	0.763080
37	6	0	3.212045	-0.426321	1.008114
38	6	0	4.466078	-1.034422	1.091927
39	6	0	4.827006	-1.962294	0.106410
40	1	0	5.146797	-0.787948	1.900751
41	6	0	2.717964	-1.587260	-0.966165
42	6	0	3.949230	-2.242854	-0.943783
43	1	0	5.796367	-2.449482	0.153956
44	1	0	4.189302	-2.942966	-1.736029
45	6	0	-3.209746	-0.433984	-1.004913
46	6	0	-4.462438	-1.045281	-1.084525
47	6	0	-2.707975	-1.589113	0.970943
48	6	0	-4.819471	-1.970321	-0.094869
49	1	0	-5.145357	-0.802835	-1.892718
50	6	0	-3.939428	-2.244526	0.954984
51	1	0	-5.788018	-2.459480	-0.138613
52	1	0	-4.177254	-2.939885	1.752072
53	7	0	-2.364224	-0.724014	-0.000929
54	7	0	2.370022	-0.719761	0.002199
55	6	0	1.670084	-1.803434	-2.059294
56	8	0	0.668232	-0.962700	-2.007628
57	8	0	1.828753	-2.727706	-2.850488
58	6	0	-1.661528	-1.798852	2.066958
59	8	0	-1.842746	-2.690087	2.889642
60	8	0	-0.639326	-0.983443	1.989113
61	7	0	-1.087830	1.720725	1.532135
62	7	0	1.081633	1.734443	-1.530904
63	1	0	-1.806910	1.079169	1.872153

64	1	0	1.800903	1.093787	-1.872462

E(RTPSSh) = -1598.95130615

Zero-point correction= 0.529592 (Hartree/Particle)

Thermal correction to Energy= 0.560787

Thermal correction to Enthalpy= 0.561731

Thermal correction to Gibbs Free Energy= 0.470772

Sum of electronic and zero-point Energies= -1598.425514

Sum of electronic and thermal Energies= -1598.394320

Sum of electronic and thermal Enthalpies= -1598.393376

Sum of electronic and thermal Free Energies= -1598.484334

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.002309	-0.082241	-0.037920
2	7	0	1.538965	1.466346	-1.538995
3	6	0	2.184802	2.565675	-0.754194
4	6	0	2.597653	2.166779	0.660799
5	6	0	0.709569	2.510435	2.235877
6	6	0	-0.553761	1.837362	2.765209
7	7	0	-1.433948	1.339808	1.662896
8	6	0	-2.075314	2.518222	0.992796
9	6	0	-2.485127	2.287855	-0.462161
10	6	0	-0.577668	2.730568	-2.017311
11	6	0	0.674479	2.069978	-2.599576
12	6	0	2.573877	0.592872	-2.166040
13	6	0	-2.456979	0.428649	2.251623
14	8	0	0.075198	-2.596788	-0.186707
15	1	0	1.464315	3.381569	-0.679039
16	1	0	3.053581	2.953934	-1.304503
17	1	0	3.417843	1.448518	0.648418
18	1	0	2.964144	3.062388	1.179358
19	1	0	0.482458	3.403129	1.647401

20	1	0	1.316854	2.839158	3.090518
21	1	0	-0.264581	0.968963	3.364464
22	1	0	-1.103395	2.530733	3.417544
23	1	0	-1.350358	3.333326	1.012551
24	1	0	-2.945734	2.848670	1.576754
25	1	0	-3.323261	1.593853	-0.532187
26	1	0	-2.826886	3.245311	-0.876582
27	1	0	-0.329408	3.563242	-1.354342
28	1	0	-1.167783	3.148044	-2.844381
29	1	0	0.368175	1.258964	-3.267927
30	1	0	1.237952	2.803073	-3.194340
31	1	0	2.078865	0.006438	-2.949440
32	1	0	3.355870	1.192159	-2.651681
33	1	0	-1.935059	-0.246749	2.939898
34	1	0	-3.193638	0.992418	2.840366
35	1	0	-0.288626	-3.048548	-0.968163
36	1	0	-0.218245	-3.103366	0.591081
37	6	0	3.188440	-0.364958	-1.162819
38	6	0	4.500215	-0.840330	-1.257764
39	6	0	4.963504	-1.729722	-0.284602
40	1	0	5.143766	-0.513572	-2.067700
41	6	0	2.832105	-1.579205	0.803222
42	6	0	4.123941	-2.101882	0.769308
43	1	0	5.978087	-2.111903	-0.338092
44	1	0	4.449488	-2.767075	1.560430
45	6	0	-3.153837	-0.402416	1.196131
46	6	0	-4.480450	-0.830192	1.308569
47	6	0	-2.945543	-1.418839	-0.894661
48	6	0	-5.028112	-1.599679	0.279156
49	1	0	-5.070854	-0.557178	2.176756
50	6	0	-4.255204	-1.893403	-0.847275
51	1	0	-6.055202	-1.944417	0.345522
52	1	0	-4.645498	-2.457580	-1.686120
53	7	0	-2.407834	-0.717695	0.123251
54	7	0	2.383160	-0.750726	-0.158738
55	6	0	1.861848	-1.859825	1.945941

56	8	0	0.759634	-1.167968	1.910853
57	8	0	2.187163	-2.677716	2.814320
58	6	0	-2.054341	-1.598537	-2.116875
59	8	0	-2.450373	-2.315433	-3.044334
60	8	0	-0.935307	-0.940184	-2.069355
61	7	0	-1.357123	1.734556	-1.249617
62	7	0	1.451790	1.562052	1.379521
63	1	0	1.803216	0.826065	1.993365
64	1	0	-1.730920	1.068458	-1.927899

E(RTPSSh) = -1598.95760332

Zero-point correction= 0.529710 (Hartree/Particle)

Thermal correction to Energy= 0.561140

Thermal correction to Enthalpy= 0.562084

Thermal correction to Gibbs Free Energy= 0.470343

Sum of electronic and zero-point Energies= -1598.427923

Sum of electronic and thermal Energies= -1598.396493

Sum of electronic and thermal Enthalpies= -1598.395549

Sum of electronic and thermal Free Energies= -1598.487290

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000000	0.020667	-0.000007
2	7	0	-1.642873	-1.214409	1.622940
3	6	0	-0.816703	-1.786879	2.720906
4	6	0	0.316868	-2.678519	2.211242
5	6	0	1.816764	-2.938853	0.263517
6	6	0	2.486528	-2.224337	-0.916073
7	7	0	1.642885	-1.214403	-1.622941
8	6	0	0.816720	-1.786879	-2.720908
9	6	0	-0.316847	-2.678525	-2.211243
10	6	0	-1.816744	-2.938864	-0.263517
11	6	0	-2.486511	-2.224348	0.916071

12	6	0	-2.536135	-0.157261	2.183692
13	6	0	2.536142	-0.157247	-2.183687
14	8	0	0.000045	2.566382	-0.000027
15	1	0	-1.440956	-2.364766	3.421035
16	1	0	-0.387007	-0.937283	3.257612
17	1	0	1.078413	-3.665552	-0.081534
18	1	0	2.592460	-3.511799	0.793873
19	1	0	3.363128	-1.693460	-0.533663
20	1	0	2.856480	-2.977469	-1.628124
21	1	0	1.440977	-2.364764	-3.421034
22	1	0	0.387020	-0.937286	-3.257618
23	1	0	-1.078390	-3.665559	0.081535
24	1	0	-2.592437	-3.511815	-0.793871
25	1	0	-3.363112	-1.693475	0.533659
26	1	0	-2.856462	-2.977480	1.628123
27	1	0	-3.316617	-0.587962	2.828300
28	1	0	-1.910746	0.497892	2.801557
29	1	0	3.316629	-0.587940	-2.828294
30	1	0	1.910751	0.497905	-2.801553
31	1	0	-0.070424	3.138145	-0.783828
32	1	0	0.070236	3.138125	0.783813
33	6	0	-3.149646	0.651949	1.055824
34	6	0	-4.405452	1.261906	1.097692
35	6	0	-4.826815	2.001806	-0.014382
36	1	0	-5.038661	1.162167	1.973813
37	6	0	-2.759929	1.468163	-1.102202
38	6	0	-3.998048	2.110248	-1.134200
39	1	0	-5.799742	2.484138	-0.004578
40	1	0	-4.278340	2.670994	-2.018873
41	6	0	3.149643	0.651963	-1.055813
42	6	0	4.405442	1.261933	-1.097676
43	6	0	2.759911	1.468168	1.102213
44	6	0	4.826796	2.001834	0.014401
45	1	0	5.038653	1.162206	-1.973797
46	6	0	3.998025	2.110263	1.134218
47	1	0	5.799718	2.484175	0.004601

48	1	0	4.278309	2.671007	2.018893
49	7	0	2.363233	0.762723	0.028015
50	7	0	-2.363239	0.762722	-0.028005
51	6	0	-1.752727	1.536856	-2.248836
52	8	0	-0.679198	0.811390	-2.051406
53	8	0	-2.003980	2.246763	-3.215900
54	6	0	1.752706	1.536854	2.248843
55	8	0	2.003973	2.246720	3.215933
56	8	0	0.679155	0.811426	2.051386
57	1	0	-0.943997	-2.968962	-3.064403
58	1	0	0.076704	-3.606255	-1.788029
59	1	0	-0.076677	-3.606251	1.788028
60	1	0	0.944021	-2.968952	3.064401
61	7	0	-1.114144	-1.995511	-1.157174
62	7	0	1.114159	-1.995500	1.157172
63	1	0	-1.802781	-1.403306	-1.628889
64	1	0	1.802797	-1.403294	1.628885

E(RTPSSh) = -1598.96184573

Zero-point correction= 0.529352 (Hartree/Particle)

Thermal correction to Energy= 0.560963

Thermal correction to Enthalpy= 0.561908

Thermal correction to Gibbs Free Energy= 0.469839

Sum of electronic and zero-point Energies= -1598.434901

Sum of electronic and thermal Energies= -1598.403290

Sum of electronic and thermal Enthalpies= -1598.402346

Sum of electronic and thermal Free Energies= -1598.494415

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.712087	-1.836953	-0.803196
2	6	0	1.096264	-2.740252	-1.830052
3	6	0	0.065141	-2.036563	-2.710398

4	6	0	-2.130148	-2.190217	-1.467688
5	6	0	-1.872939	-2.868219	-0.120752
6	7	0	-1.525514	-1.927306	0.986444
7	6	0	-0.786808	-2.651164	2.067112
8	6	0	0.096530	-1.697112	2.861891
9	6	0	2.281508	-1.846371	1.675553
10	6	0	2.134202	-2.647626	0.380667
11	6	0	2.909498	-1.179429	-1.402297
12	6	0	-2.754435	-1.385105	1.629366
13	1	0	0.628973	-3.574259	-1.304896
14	1	0	1.872792	-3.176517	-2.472899
15	1	0	-3.008846	-1.545079	-1.404836
16	1	0	-2.351415	-2.974135	-2.204797
17	1	0	-2.757483	-3.465008	0.144983
18	1	0	-1.042451	-3.568710	-0.219651
19	1	0	-0.180472	-3.433277	1.611378
20	1	0	-1.488223	-3.157504	2.744505
21	1	0	3.143495	-1.180988	1.620269
22	1	0	2.481027	-2.557753	2.488684
23	1	0	3.085207	-3.158795	0.171843
24	1	0	1.387909	-3.429639	0.519633
25	1	0	3.729475	-1.904865	-1.497167
26	1	0	2.642073	-0.858444	-2.413701
27	1	0	-3.495344	-2.186693	1.757677
28	1	0	-2.479634	-1.050170	2.635669
29	6	0	3.377916	0.028474	-0.617548
30	6	0	4.716918	0.430422	-0.576631
31	6	0	5.052625	1.588435	0.130210
32	1	0	5.477417	-0.153936	-1.083730
33	6	0	2.740691	1.841683	0.708812
34	6	0	4.052151	2.308563	0.786632
35	1	0	6.085993	1.917602	0.173653
36	1	0	4.262444	3.206985	1.354828
37	6	0	-3.381415	-0.206773	0.933701
38	6	0	-4.742100	0.082614	1.099979
39	6	0	-3.080955	1.687842	-0.359181

40	6	0	-5.261481	1.242591	0.528932
41	1	0	-5.372542	-0.590836	1.671283
42	6	0	-4.412879	2.066008	-0.213519
43	1	0	-6.310631	1.492657	0.650618
44	1	0	-4.757971	2.974110	-0.693856
45	7	0	-2.566559	0.581436	0.214835
46	7	0	2.421241	0.731802	0.016171
47	6	0	1.577018	2.533414	1.403948
48	8	0	0.434397	1.929995	1.263601
49	8	0	1.789310	3.573907	2.035570
50	6	0	-2.127345	2.466111	-1.230081
51	8	0	-2.468613	3.547994	-1.715146
52	8	0	-0.991947	1.859404	-1.413833
53	1	0	0.594050	-2.253934	3.667696
54	1	0	-0.508582	-0.914494	3.330202
55	1	0	0.551710	-1.269653	-3.315897
56	1	0	-0.374314	-2.780564	-3.388873
57	7	0	1.084849	-1.018621	1.987042
58	7	0	-0.997611	-1.340874	-1.929852
59	1	0	1.412426	-0.200093	2.500752
60	1	0	-1.400829	-0.646289	-2.561629
61	67	0	-0.004573	0.122980	-0.105860
62	8	0	1.007486	0.842534	-2.412935
63	1	0	1.832058	1.357859	-2.365151
64	1	0	0.283805	1.521749	-2.454068

E(RTPSSh) = -1598.95165012

Zero-point correction= 0.531043 (Hartree/Particle)

Thermal correction to Energy= 0.561926

Thermal correction to Enthalpy= 0.562870

Thermal correction to Gibbs Free Energy= 0.471264

Sum of electronic and zero-point Energies= -1598.421160

Sum of electronic and thermal Energies= -1598.390276

Sum of electronic and thermal Enthalpies= -1598.389332

Sum of electronic and thermal Free Energies= -1598.480938

[Yb(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	-0.001257	0.006435	-0.003607
2	7	0	1.741199	1.533022	1.310921
3	6	0	1.073960	2.482117	2.251159
4	6	0	-0.299575	1.992924	2.691256
5	6	0	-1.768202	2.832544	0.840795
6	6	0	-2.590787	2.315707	-0.336191
7	7	0	-1.743348	1.544785	-1.299032
8	6	0	-1.077792	2.505001	-2.229123
9	6	0	0.296951	2.022925	-2.674583
10	6	0	1.764192	2.844608	-0.814713
11	6	0	2.587447	2.315876	0.356727
12	6	0	2.584207	0.546406	2.044805
13	6	0	-2.585578	0.564679	-2.042596
14	1	0	0.969812	3.438114	1.730895
15	1	0	1.707336	2.667132	3.128807
16	1	0	-0.214310	1.067759	3.266491
17	1	0	-0.766158	2.752910	3.332913
18	1	0	-0.981769	3.514234	0.504028
19	1	0	-2.419071	3.398767	1.520917
20	1	0	-3.372429	1.652733	0.045268
21	1	0	-3.092636	3.145632	-0.850393
22	1	0	-0.975400	3.455564	-1.698685
23	1	0	-1.711385	2.698203	-3.104840
24	1	0	0.213455	1.104068	-3.260184
25	1	0	0.762273	2.790630	-3.307880
26	1	0	0.976501	3.521130	-0.470607
27	1	0	2.414299	3.419531	-1.488234
28	1	0	3.370185	1.658546	-0.032251

29	1	0	3.088198	3.140770	0.880034
30	1	0	3.415963	1.037505	2.568672
31	1	0	1.954118	0.062097	2.800250
32	1	0	-3.419166	1.060334	-2.559236
33	1	0	-1.955925	0.091007	-2.805156
34	6	0	3.115267	-0.488517	1.069502
35	6	0	4.366148	-1.103719	1.170037
36	6	0	4.758234	-1.991810	0.163358
37	1	0	5.021667	-0.881312	2.005180
38	6	0	2.681394	-1.578046	-0.958670
39	6	0	3.915817	-2.224103	-0.928165
40	1	0	5.726397	-2.479386	0.219733
41	1	0	4.196489	-2.878913	-1.744672
42	6	0	-3.112640	-0.482630	-1.078026
43	6	0	-4.360506	-1.101962	-1.186900
44	6	0	-2.674515	-1.592340	0.938377
45	6	0	-4.749844	-2.001209	-0.189006
46	1	0	-5.016018	-0.873943	-2.020570
47	6	0	-3.907810	-2.240376	0.900932
48	1	0	-5.716301	-2.491666	-0.250765
49	1	0	-4.187747	-2.902825	1.711531
50	7	0	-2.296060	-0.755772	-0.045891
51	7	0	2.299165	-0.754553	0.035275
52	6	0	1.688353	-1.720361	-2.109351
53	8	0	0.618645	-0.990274	-2.002211
54	8	0	1.963100	-2.492858	-3.035972
55	6	0	-1.688103	-1.739819	2.092025
56	8	0	-1.978381	-2.493678	3.028431
57	8	0	-0.611169	-1.018226	1.986777
58	7	0	-1.144399	1.676485	1.514701
59	7	0	1.142456	1.694997	-1.501662
60	1	0	-1.900400	1.079374	1.854152
61	1	0	1.899426	1.103268	-1.848206
62	8	0	-0.053730	-2.634880	0.033163
63	1	0	0.348736	-3.046385	0.818019
64	1	0	0.151337	-3.236114	-0.704318

E(RTPSSh) = -1600.70049397

Zero-point correction= 0.529458 (Hartree/Particle)

Thermal correction to Energy= 0.560791

Thermal correction to Enthalpy= 0.561735

Thermal correction to Gibbs Free Energy= 0.470371

Sum of electronic and zero-point Energies= -1600.171113

Sum of electronic and thermal Energies= -1600.139780

Sum of electronic and thermal Enthalpies= -1600.138836

Sum of electronic and thermal Free Energies= -1600.230200

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.526683	1.409206	1.585203
2	6	0	-2.205334	2.530064	0.865740
3	6	0	-2.529616	2.240163	-0.602769
4	6	0	-0.577208	2.663882	-2.110452
5	6	0	0.669403	1.972985	-2.670152
6	7	0	1.526683	1.408849	-1.585519
7	6	0	2.205397	2.529765	-0.866205
8	6	0	2.529685	2.240052	0.602338
9	6	0	0.577306	2.664135	2.109919
10	6	0	-0.669344	1.973429	2.669739
11	6	0	-2.515651	0.458382	2.170310
12	6	0	2.515599	0.457840	-2.170431
13	8	0	0.000796	-2.598183	-0.000276
14	1	0	-1.533137	3.390327	0.900296
15	1	0	-3.121442	2.822592	1.400445
16	1	0	-3.339913	1.514804	-0.687450
17	1	0	-2.882216	3.169751	-1.070498
18	1	0	-0.320705	3.519721	-1.477329
19	1	0	-1.168778	3.056118	-2.950669
20	1	0	0.353506	1.135890	-3.300127

21	1	0	1.237324	2.677068	-3.296839
22	1	0	1.533243	3.390057	-0.900876
23	1	0	3.121516	2.822173	-1.400953
24	1	0	3.339950	1.514673	0.687113
25	1	0	2.882319	3.169694	1.069937
26	1	0	0.320869	3.519862	1.476619
27	1	0	1.168901	3.056498	2.950057
28	1	0	-0.353498	1.136397	3.299826
29	1	0	-1.237198	2.677647	3.296337
30	1	0	-1.967834	-0.183354	2.871151
31	1	0	-3.291986	0.991303	2.739308
32	1	0	1.967747	-0.184007	-2.871145
33	1	0	3.291966	0.990599	-2.739535
34	1	0	0.042080	-3.169916	0.786538
35	1	0	-0.044888	-3.170456	-0.786472
36	6	0	-3.140702	-0.420985	1.103626
37	6	0	-4.446154	-0.915855	1.149415
38	6	0	-4.884235	-1.747394	0.111441
39	1	0	-5.105083	-0.658835	1.972870
40	6	0	-2.743745	-1.501136	-0.935842
41	6	0	-4.026519	-2.048681	-0.949965
42	1	0	-5.894101	-2.146266	0.128828
43	1	0	-4.321938	-2.680359	-1.780147
44	6	0	3.140589	-0.421329	-1.103534
45	6	0	4.445989	-0.916344	-1.149228
46	6	0	2.743585	-1.500826	0.936271
47	6	0	4.884034	-1.747568	-0.110988
48	1	0	5.104904	-0.659659	-1.972799
49	6	0	4.026350	-2.048381	0.950573
50	1	0	5.893866	-2.146536	-0.128281
51	1	0	4.321754	-2.679739	1.781003
52	7	0	2.323954	-0.725621	-0.081134
53	7	0	-2.324070	-0.725634	0.081325
54	6	0	-1.726118	-1.724740	-2.054154
55	8	0	-0.682648	-0.930901	-1.986522
56	8	0	-1.945146	-2.593536	-2.890078

57	6	0	1.726147	-1.723882	2.054862
58	8	0	1.946037	-2.591165	2.892100
59	8	0	0.681953	-0.931006	1.986234
60	7	0	1.345312	1.697661	1.302790
61	7	0	-1.345269	1.697622	-1.303126
62	1	0	-1.638990	0.949099	-1.935594
63	1	0	1.639047	0.949317	1.935447
64	70	0	-0.000021	-0.043317	-0.000123

E(RTPSSh) = -1600.70128434

Zero-point correction= 0.530057 (Hartree/Particle)

Thermal correction to Energy= 0.561331

Thermal correction to Enthalpy= 0.562275

Thermal correction to Gibbs Free Energy= 0.471182

Sum of electronic and zero-point Energies= -1600.174210

Sum of electronic and thermal Energies= -1600.142936

Sum of electronic and thermal Enthalpies= -1600.141992

Sum of electronic and thermal Free Energies= -1600.233085

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	-0.000737	-0.000876	-0.006853
2	7	0	-1.638578	1.200194	-1.621514
3	6	0	-0.821534	1.783142	-2.720061
4	6	0	0.309968	2.673897	-2.204591
5	6	0	1.807364	2.931919	-0.256020
6	6	0	2.474575	2.214092	0.922384
7	7	0	1.624310	1.205027	1.622199
8	6	0	0.800725	1.778068	2.721312
9	6	0	-0.335639	2.662752	2.208544
10	6	0	-1.831592	2.918154	0.261614
11	6	0	-2.494969	2.202008	-0.919111
12	6	0	-2.518410	0.129214	-2.176043

13	6	0	2.510266	0.142163	2.182175
14	8	0	-0.048899	-2.541967	-0.032678
15	1	0	-1.451134	2.365257	-3.411664
16	1	0	-0.391381	0.939796	-3.265191
17	1	0	1.070201	3.659791	0.089269
18	1	0	2.583213	3.503223	-0.787572
19	1	0	3.350595	1.681938	0.540078
20	1	0	2.845086	2.963725	1.637651
21	1	0	1.425257	2.360335	3.417362
22	1	0	0.374932	0.928539	3.260545
23	1	0	-1.097689	3.650868	-0.080400
24	1	0	-2.609703	3.483517	0.796168
25	1	0	-3.368753	1.664424	-0.539647
26	1	0	-2.868051	2.952312	-1.632270
27	1	0	-3.307955	0.545952	-2.818590
28	1	0	-1.885320	-0.520250	-2.791642
29	1	0	3.294625	0.566358	2.826242
30	1	0	1.879049	-0.509934	2.796771
31	1	0	0.085331	-3.082202	0.765081
32	1	0	0.141403	-3.101118	-0.806024
33	6	0	-3.112224	-0.680944	-1.039217
34	6	0	-4.356717	-1.314330	-1.067395
35	6	0	-4.758767	-2.049225	0.054815
36	1	0	-4.996112	-1.235644	-1.941129
37	6	0	-2.693461	-1.472411	1.121867
38	6	0	-3.921385	-2.131737	1.170413
39	1	0	-5.723209	-2.548375	0.055997
40	1	0	-4.186756	-2.687039	2.063046
41	6	0	3.114840	-0.666622	1.050917
42	6	0	4.367328	-1.284451	1.083069
43	6	0	2.714783	-1.461842	-1.112774
44	6	0	4.781238	-2.017438	-0.036112
45	1	0	5.004069	-1.194600	1.957666
46	6	0	3.948718	-2.110724	-1.154811
47	1	0	5.751551	-2.505082	-0.033495
48	1	0	4.223789	-2.663920	-2.045886

49	7	0	2.323219	-0.765363	-0.030340
50	7	0	-2.316813	-0.767937	0.039843
51	6	0	-1.675028	-1.516830	2.257235
52	8	0	-0.593649	-0.811946	2.021215
53	8	0	-1.921472	-2.184327	3.254522
54	6	0	1.701935	-1.509147	-2.254390
55	8	0	1.935413	-2.218705	-3.226408
56	8	0	0.642323	-0.767794	-2.045437
57	1	0	-0.969642	2.949079	3.057894
58	1	0	0.053217	3.593044	1.786547
59	1	0	-0.085070	3.600355	-1.779954
60	1	0	0.941557	2.966868	-3.053463
61	7	0	-1.123043	1.973768	1.150347
62	7	0	1.103278	1.988156	-1.148420
63	1	0	-1.811841	1.380191	1.619831
64	1	0	1.791883	1.396663	-1.620932

E(RTPSSh) = -1600.70927828

Zero-point correction= 0.529950 (Hartree/Particle)

Thermal correction to Energy= 0.561334

Thermal correction to Enthalpy= 0.562278

Thermal correction to Gibbs Free Energy= 0.471064

Sum of electronic and zero-point Energies= -1600.181557

Sum of electronic and thermal Energies= -1600.150173

Sum of electronic and thermal Enthalpies= -1600.149229

Sum of electronic and thermal Free Energies= -1600.240443

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.646370	-1.834796	-0.890285
2	6	0	0.988954	-2.698652	-1.927924
3	6	0	-0.074580	-1.957043	-2.734296
4	6	0	-2.193432	-2.153800	-1.387445

5	6	0	-1.863970	-2.840218	-0.060561
6	7	0	-1.492791	-1.900066	1.037287
7	6	0	-0.752903	-2.618599	2.122814
8	6	0	0.179158	-1.666157	2.862161
9	6	0	2.298649	-1.908660	1.568853
10	6	0	2.076485	-2.679746	0.266022
11	6	0	2.843047	-1.183349	-1.499891
12	6	0	-2.715030	-1.336619	1.678666
13	1	0	0.546871	-3.565208	-1.418589
14	1	0	1.743149	-3.110789	-2.623821
15	1	0	-3.093468	-1.531361	-1.282065
16	1	0	-2.429315	-2.939526	-2.129107
17	1	0	-2.725447	-3.469483	0.237781
18	1	0	-1.014483	-3.521360	-0.201288
19	1	0	-0.180872	-3.442417	1.678334
20	1	0	-1.458213	-3.085396	2.835162
21	1	0	3.195722	-1.278655	1.500881
22	1	0	2.495044	-2.647031	2.368424
23	1	0	3.002151	-3.234370	0.016282
24	1	0	1.297913	-3.438073	0.418332
25	1	0	3.660751	-1.920870	-1.613014
26	1	0	2.565983	-0.862135	-2.517441
27	1	0	-3.454669	-2.140735	1.856497
28	1	0	-2.424080	-0.955779	2.672857
29	6	0	3.338437	0.013031	-0.713495
30	6	0	4.681113	0.416775	-0.708949
31	6	0	5.044843	1.553513	0.024584
32	1	0	5.426044	-0.156792	-1.264155
33	6	0	2.752161	1.782913	0.705883
34	6	0	4.069659	2.248339	0.748485
35	1	0	6.086185	1.883183	0.039574
36	1	0	4.298309	3.129760	1.349318
37	6	0	-3.352035	-0.191805	0.939141
38	6	0	-4.729013	0.061027	1.033759
39	6	0	-3.039511	1.701911	-0.369240
40	6	0	-5.256059	1.195280	0.409990

41	1	0	-5.369365	-0.625229	1.591520
42	6	0	-4.394378	2.034840	-0.302275
43	1	0	-6.324339	1.414311	0.472783
44	1	0	-4.739052	2.931936	-0.818288
45	7	0	-2.519656	0.611209	0.244061
46	7	0	2.402025	0.698427	-0.020210
47	6	0	1.619737	2.439891	1.489975
48	8	0	0.475548	1.813723	1.396709
49	8	0	1.855722	3.467012	2.144912
50	6	0	-2.062921	2.534377	-1.170553
51	8	0	-2.439960	3.569015	-1.738763
52	8	0	-0.855423	2.031192	-1.185363
53	1	0	0.692701	-2.213404	3.674726
54	1	0	-0.396834	-0.850376	3.329495
55	1	0	0.399537	-1.173151	-3.340677
56	1	0	-0.556613	-2.677750	-3.420884
57	7	0	1.146713	-1.038594	1.929951
58	7	0	-1.095683	-1.276400	-1.881991
59	1	0	1.517253	-0.203201	2.396421
60	1	0	-1.533892	-0.565416	-2.481828
61	1	0	0.261779	1.580697	-2.344253
62	8	0	0.907571	0.815676	-2.404648
63	1	0	1.789336	1.243548	-2.382407
64	70	0	-0.002644	0.122145	-0.072704

E(RTPSSh) = -1600.69477727

Zero-point correction= 0.531528 (Hartree/Particle)

Thermal correction to Energy= 0.562260

Thermal correction to Enthalpy= 0.563204

Thermal correction to Gibbs Free Energy= 0.472111

Sum of electronic and zero-point Energies= -1600.165197

Sum of electronic and thermal Energies= -1600.134465

Sum of electronic and thermal Enthalpies= -1600.133521

Sum of electronic and thermal Free Energies= -1600.224614

[Lu(dodpa)(H_2O)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	-0.099172	-0.275582	0.043809
2	7	0	-2.327663	-1.475474	0.529034
3	6	0	-2.089911	-2.760043	1.253550
4	6	0	-0.882431	-2.681802	2.185920
5	6	0	0.961504	-3.392074	0.654866
6	6	0	2.091348	-2.833904	-0.206822
7	7	0	1.616552	-1.774785	-1.154870
8	6	0	1.020507	-2.398746	-2.374188
9	6	0	-0.002497	-1.483267	-3.044716
10	6	0	-2.114485	-2.150921	-1.886518
11	6	0	-3.052872	-1.730833	-0.758467
12	6	0	-3.145329	-0.549308	1.363912
13	6	0	2.769850	-0.907305	-1.529485
14	1	0	-1.927886	-3.535981	0.500878
15	1	0	-2.981113	-3.052295	1.824422
16	1	0	-1.038236	-1.921581	2.957040
17	1	0	-0.755721	-3.647354	2.692299
18	1	0	0.186900	-3.850611	0.033997
19	1	0	1.358461	-4.177830	1.309792
20	1	0	2.843512	-2.382201	0.446524
21	1	0	2.581941	-3.644977	-0.760529
22	1	0	0.537670	-3.329612	-2.066069
23	1	0	1.805358	-2.669916	-3.092128
24	1	0	0.469183	-0.552834	-3.373859
25	1	0	-0.406964	-1.983915	-3.933830
26	1	0	-1.609564	-3.090595	-1.644572
27	1	0	-2.698658	-2.323725	-2.799047
28	1	0	-3.556318	-0.803479	-1.045777
29	1	0	-3.829822	-2.491975	-0.609539

30	1	0	-4.170051	-0.926782	1.480436
31	1	0	-2.696164	-0.502185	2.362401
32	1	0	3.613182	-1.510477	-1.891635
33	1	0	2.452950	-0.257325	-2.352801
34	6	0	-3.150525	0.840090	0.758312
35	6	0	-4.196361	1.756280	0.905646
36	6	0	-4.071066	3.017343	0.316650
37	1	0	-5.086564	1.486189	1.463530
38	6	0	-1.922525	2.367185	-0.514766
39	6	0	-2.918059	3.335041	-0.408345
40	1	0	-4.871230	3.743686	0.416422
41	1	0	-2.783430	4.299252	-0.884068
42	6	0	3.189290	-0.046185	-0.355141
43	6	0	4.485612	0.439448	-0.162539
44	6	0	2.443438	1.019680	1.587321
45	6	0	4.740383	1.247557	0.949424
46	1	0	5.274885	0.188458	-0.862999
47	6	0	3.708520	1.541730	1.845540
48	1	0	5.739557	1.636226	1.118543
49	1	0	3.863885	2.155295	2.725216
50	7	0	2.205058	0.249260	0.509584
51	7	0	-2.049642	1.155581	0.058313
52	6	0	-0.616709	2.569718	-1.259755
53	8	0	0.172885	1.543565	-1.253057
54	8	0	-0.390623	3.661693	-1.806496
55	6	0	1.235281	1.266647	2.476708
56	8	0	1.369032	1.917716	3.515547
57	8	0	0.127120	0.742588	2.027914
58	7	0	0.344921	-2.292991	1.440743
59	7	0	-1.082323	-1.104039	-2.094107
60	1	0	1.033732	-1.984279	2.130290
61	1	0	-1.551412	-0.282685	-2.482405
62	8	0	2.382566	3.782940	-2.347164
63	1	0	2.704087	3.964156	-1.448039
64	1	0	1.405064	3.726779	-2.222384

E(RTPSSh) = -1601.26912592

Zero-point correction= 0.529020 (Hartree/Particle)

Thermal correction to Energy= 0.560845

Thermal correction to Enthalpy= 0.561789

Thermal correction to Gibbs Free Energy= 0.467178

Sum of electronic and zero-point Energies= -1600.740123

Sum of electronic and thermal Energies= -1600.708298

Sum of electronic and thermal Enthalpies= -1600.707354

Sum of electronic and thermal Free Energies= -1600.801965

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	-0.000031	-0.035822	-0.000210
2	7	0	1.522957	1.404993	-1.585982
3	6	0	2.207666	2.524575	-0.870472
4	6	0	2.530237	2.236058	0.598431
5	6	0	0.578032	2.663744	2.105139
6	6	0	-0.666219	1.972224	2.668874
7	7	0	-1.522947	1.405668	1.585386
8	6	0	-2.207547	2.525130	0.869588
9	6	0	-2.530105	2.236245	-0.599250
10	6	0	-0.577846	2.663243	-2.106149
11	6	0	0.666336	1.971373	-2.669655
12	6	0	2.506431	0.448040	-2.169997
13	6	0	-2.506511	0.449058	2.169773
14	8	0	0.001447	-2.594418	-0.000382
15	1	0	1.539833	3.388165	-0.907151
16	1	0	3.125077	2.810964	-1.406189
17	1	0	3.339274	1.509444	0.684617
18	1	0	2.883530	3.165314	1.066156
19	1	0	0.319144	3.518084	1.470963
20	1	0	1.172257	3.057571	2.942662
21	1	0	-0.348274	1.136438	3.299371

22	1	0	-1.234618	2.676331	3.295036
23	1	0	-1.539639	3.388671	0.906041
24	1	0	-3.124939	2.811744	1.405218
25	1	0	-3.339203	1.509669	-0.685254
26	1	0	-2.883331	3.165396	-1.067233
27	1	0	-0.318842	3.517798	-1.472308
28	1	0	-1.172027	3.056825	-2.943821
29	1	0	0.348300	1.135463	-3.299940
30	1	0	1.234854	2.675231	-3.295987
31	1	0	1.954272	-0.193307	-2.867664
32	1	0	3.285067	0.975208	-2.741129
33	1	0	-1.954408	-0.192087	2.867667
34	1	0	-3.285087	0.976520	2.740716
35	1	0	-0.027408	-3.167078	-0.786941
36	1	0	0.022058	-3.166067	0.787135
37	6	0	3.126862	-0.430816	-1.100430
38	6	0	4.429541	-0.933301	-1.143096
39	6	0	4.862409	-1.762198	-0.100851
40	1	0	5.090329	-0.683750	-1.967356
41	6	0	2.722339	-1.500397	0.943235
42	6	0	4.002447	-2.053750	0.961539
43	1	0	5.870126	-2.166582	-0.115658
44	1	0	4.294101	-2.682609	1.795188
45	6	0	-3.127060	-0.430170	1.100602
46	6	0	-4.429840	-0.932386	1.143449
47	6	0	-2.722643	-1.500954	-0.942457
48	6	0	-4.862784	-1.761854	0.101691
49	1	0	-5.090646	-0.682218	1.967508
50	6	0	-4.002774	-2.054274	-0.960427
51	1	0	-5.870570	-2.166057	0.116682
52	1	0	-4.294443	-2.683757	-1.793601
53	7	0	-2.308027	-0.727056	0.077996
54	7	0	2.307820	-0.727035	-0.077651
55	6	0	1.701785	-1.713543	2.060566
56	8	0	0.657759	-0.921028	1.981458
57	8	0	1.918707	-2.572510	2.906949

58	6	0	-1.701753	-1.715117	-2.059296
59	8	0	-1.917177	-2.576802	-2.903351
60	8	0	-0.658981	-0.920918	-1.981945
61	7	0	-1.343721	1.695709	-1.297910
62	7	0	1.343808	1.695811	1.297274
63	1	0	1.635821	0.947846	1.930898
64	1	0	-1.635705	0.947413	-1.931183

E(RTPSSh) = -1601.25601176

Zero-point correction= 0.530258 (Hartree/Particle)

Thermal correction to Energy= 0.561437

Thermal correction to Enthalpy= 0.562381

Thermal correction to Gibbs Free Energy= 0.471648

Sum of electronic and zero-point Energies= -1600.728689

Sum of electronic and thermal Energies= -1600.697510

Sum of electronic and thermal Enthalpies= -1600.696566

Sum of electronic and thermal Free Energies= -1600.787299

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	-0.000567	0.006217	-0.006525
2	7	0	1.625831	1.204723	1.617124
3	6	0	0.806795	1.780802	2.717831
4	6	0	-0.331691	2.662611	2.205290
5	6	0	-1.833164	2.914466	0.263719
6	6	0	-2.497581	2.197275	-0.915407
7	7	0	-1.639478	1.197248	-1.618140
8	6	0	-0.826984	1.782048	-2.718856
9	6	0	0.306221	2.670987	-2.204651
10	6	0	1.808911	2.928466	-0.261849
11	6	0	2.477488	2.211423	0.915807
12	6	0	2.510442	0.139986	2.175078
13	6	0	-2.517561	0.123712	-2.169939

14	8	0	-0.043699	-2.534161	-0.027302
15	1	0	1.433649	2.366025	3.409249
16	1	0	0.383680	0.933034	3.261599
17	1	0	-1.102396	3.649715	-0.079789
18	1	0	-2.610921	3.476806	0.801894
19	1	0	-3.369610	1.657960	-0.534336
20	1	0	-2.873445	2.946426	-1.628259
21	1	0	-1.459000	2.365867	-3.406760
22	1	0	-0.399132	0.939797	-3.267176
23	1	0	1.074578	3.659024	0.084016
24	1	0	2.584119	3.496378	-0.797876
25	1	0	3.351998	1.677418	0.532615
26	1	0	2.850423	2.960969	1.629843
27	1	0	3.298773	0.562193	2.815566
28	1	0	1.879380	-0.509947	2.791953
29	1	0	-3.310779	0.537708	-2.809704
30	1	0	-1.884245	-0.524154	-2.786790
31	1	0	0.119426	-3.097139	-0.803898
32	1	0	0.097208	-3.076125	0.767945
33	6	0	3.106925	-0.670707	1.041331
34	6	0	4.356253	-1.295251	1.067903
35	6	0	4.761875	-2.029579	-0.053319
36	1	0	4.996850	-1.209444	1.940078
37	6	0	2.693551	-1.463520	-1.120352
38	6	0	3.923949	-2.118387	-1.168372
39	1	0	5.729695	-2.522154	-0.055015
40	1	0	4.192001	-2.673174	-2.060596
41	6	0	-3.103798	-0.686951	-1.030059
42	6	0	-4.345625	-1.325875	-1.051916
43	6	0	-2.673077	-1.472659	1.130404
44	6	0	-4.740235	-2.060064	0.073289
45	1	0	-4.988683	-1.251771	-1.923349
46	6	0	-3.897927	-2.136912	1.185611
47	1	0	-5.702575	-2.563220	0.079337
48	1	0	-4.157078	-2.691843	2.080303
49	7	0	-2.303598	-0.768157	0.045869

50	7	0	2.310279	-0.764453	-0.036600
51	6	0	1.673036	-1.508006	-2.254422
52	8	0	0.618572	-0.761239	-2.038234
53	8	0	1.894517	-2.220590	-3.226962
54	6	0	-1.647987	-1.511650	2.259243
55	8	0	-1.882831	-2.181302	3.257856
56	8	0	-0.572615	-0.800125	2.015876
57	1	0	0.937721	2.963634	-3.053688
58	1	0	-0.087049	3.597701	-1.778898
59	1	0	0.055015	3.592791	1.781057
60	1	0	-0.965627	2.949375	3.054525
61	7	0	1.099468	1.983759	-1.149215
62	7	0	-1.118914	1.970667	1.148702
63	1	0	1.785216	1.389651	-1.622586
64	1	0	-1.804477	1.374629	1.619785

E(RTPSSh) = -1601.26389561

Zero-point correction= 0.530056 (Hartree/Particle)

Thermal correction to Energy= 0.561412

Thermal correction to Enthalpy= 0.562357

Thermal correction to Gibbs Free Energy= 0.471130

Sum of electronic and zero-point Energies= -1600.736086

Sum of electronic and thermal Energies= -1600.704730

Sum of electronic and thermal Enthalpies= -1600.703786

Sum of electronic and thermal Free Energies= -1600.795013

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.427521	-1.891260	1.148750
2	6	0	-0.724613	-2.460710	2.347707
3	6	0	0.196189	-1.435958	3.002621
4	6	0	2.401561	-1.673750	1.788482
5	6	0	2.263422	-2.609610	0.586852

6	7	0	1.813250	-1.934266	-0.673091
7	6	0	1.242048	-2.959789	-1.609862
8	6	0	0.187487	-2.364922	-2.538523
9	6	0	-1.986981	-2.529231	-1.254414
10	6	0	-1.740705	-2.993576	0.182710
11	6	0	-2.675800	-1.215890	1.622349
12	6	0	2.959101	-1.259947	-1.358565
13	1	0	-0.144003	-3.325080	2.021578
14	1	0	-1.451727	-2.830436	3.082154
15	1	0	3.224900	-0.973594	1.635281
16	1	0	2.654132	-2.281871	2.666687
17	1	0	3.219208	-3.125975	0.421852
18	1	0	1.523877	-3.379041	0.814627
19	1	0	0.796695	-3.754690	-1.009495
20	1	0	2.037709	-3.425322	-2.205426
21	1	0	-2.912680	-1.954026	-1.316939
22	1	0	-2.118120	-3.421637	-1.879875
23	1	0	-2.614142	-3.564999	0.526048
24	1	0	-0.890758	-3.678173	0.197530
25	1	0	-3.448656	-1.963048	1.845589
26	1	0	-2.439010	-0.709729	2.564981
27	1	0	3.846139	-1.906544	-1.338047
28	1	0	2.682284	-1.129252	-2.410812
29	6	0	-3.206885	-0.175349	0.661477
30	6	0	-4.556044	0.189021	0.605598
31	6	0	-4.940985	1.207271	-0.269536
32	1	0	-5.284738	-0.315138	1.231320
33	6	0	-2.661039	1.393587	-0.982418
34	6	0	-3.982051	1.822469	-1.079402
35	1	0	-5.982233	1.508057	-0.327046
36	1	0	-4.235571	2.606460	-1.783052
37	6	0	3.288324	0.107643	-0.799582
38	6	0	4.557642	0.687064	-0.909219
39	6	0	2.454804	2.016946	0.258442
40	6	0	4.747837	1.984193	-0.429504
41	1	0	5.374363	0.132889	-1.358940

42	6	0	3.681068	2.667897	0.162482
43	1	0	5.723176	2.453705	-0.507105
44	1	0	3.786630	3.671910	0.555997
45	7	0	2.272363	0.771014	-0.226141
46	7	0	-2.292668	0.425485	-0.117854
47	6	0	-1.544896	1.942138	-1.858074
48	8	0	-0.409209	1.319581	-1.725267
49	8	0	-1.782648	2.885947	-2.616975
50	6	0	1.239095	2.622516	0.933667
51	8	0	1.250405	3.822336	1.247308
52	8	0	0.262507	1.789363	1.126865
53	1	0	-0.220133	-3.163633	-3.171656
54	1	0	0.637385	-1.618588	-3.200667
55	1	0	-0.384591	-0.591671	3.387429
56	1	0	0.703470	-1.903805	3.856398
57	7	0	-0.891828	-1.669707	-1.785320
58	7	0	1.173169	-0.869754	2.035365
59	1	0	-1.318921	-1.013772	-2.439920
60	1	0	1.471039	0.027068	2.419616
61	71	0	0.045607	-0.133819	-0.065084
62	8	0	-1.484519	3.758534	1.942586
63	1	0	-0.587084	4.110257	1.748384
64	1	0	-1.297872	2.822072	1.746625

E(RTPSSh) = -1601.25465700

Zero-point correction= 0.529481 (Hartree/Particle)

Thermal correction to Energy= 0.561115

Thermal correction to Enthalpy= 0.562059

Thermal correction to Gibbs Free Energy= 0.468562

Sum of electronic and zero-point Energies= -1600.725556

Sum of electronic and thermal Energies= -1600.693922

Sum of electronic and thermal Enthalpies= -1600.692978

Sum of electronic and thermal Free Energies= -1600.786475

[La(dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	0.002589	-0.168270	-0.015074
2	7	0	1.969100	1.659613	0.972774
3	6	0	1.382386	2.654004	1.914362
4	6	0	0.198595	2.113151	2.705075
5	6	0	-1.667984	2.815993	1.222342
6	6	0	-2.656341	2.318608	0.163315
7	7	0	-1.987495	1.652719	-0.994967
8	6	0	-1.417880	2.684086	-1.908919
9	6	0	-0.216662	2.185593	-2.712190
10	6	0	1.633778	2.876797	-1.207257
11	6	0	2.624497	2.363679	-0.168533
12	6	0	2.993409	0.861918	1.697039
13	6	0	-2.987421	0.842653	-1.742153
14	1	0	1.069535	3.523338	1.332085
15	1	0	2.149328	3.011389	2.615976
16	1	0	0.493907	1.236172	3.289726
17	1	0	-0.125798	2.886587	3.415933
18	1	0	-0.954808	3.517444	0.781516
19	1	0	-2.225541	3.369873	1.990372
20	1	0	-3.332110	1.592999	0.623800
21	1	0	-3.271680	3.160767	-0.185879
22	1	0	-1.122700	3.543853	-1.303182
23	1	0	-2.189979	3.045957	-2.602861
24	1	0	-0.494242	1.322014	-3.324634
25	1	0	0.099743	2.985573	-3.396788
26	1	0	0.908975	3.553403	-0.746714
27	1	0	2.181139	3.462436	-1.958767
28	1	0	3.304478	1.654834	-0.649977
29	1	0	3.234286	3.200626	0.202257
30	1	0	3.833135	1.499415	2.010856

31	1	0	2.530165	0.467156	2.609134
32	1	0	-3.837283	1.465611	-2.058759
33	1	0	-2.505582	0.469131	-2.653388
34	6	0	3.506365	-0.288810	0.862260
35	6	0	4.819175	-0.758610	0.974498
36	6	0	5.218584	-1.837293	0.184098
37	1	0	5.510867	-0.283408	1.662231
38	6	0	3.016016	-1.875890	-0.762987
39	6	0	4.305549	-2.404199	-0.704935
40	1	0	6.232468	-2.219022	0.253104
41	1	0	4.564576	-3.233552	-1.352391
42	6	0	-3.486876	-0.329480	-0.920824
43	6	0	-4.770128	-0.864121	-1.075109
44	6	0	-3.000581	-1.839266	0.786874
45	6	0	-5.152109	-1.939401	-0.268958
46	1	0	-5.453760	-0.441489	-1.804092
47	6	0	-4.260219	-2.429765	0.687715
48	1	0	-6.141539	-2.373703	-0.373467
49	1	0	-4.516631	-3.242685	1.356868
50	7	0	-2.624347	-0.826375	-0.017416
51	7	0	2.626602	-0.845098	0.010689
52	6	0	1.972195	-2.429129	-1.716595
53	8	0	0.822572	-1.840921	-1.660829
54	8	0	2.287039	-3.372033	-2.455209
55	6	0	-1.981690	-2.278094	1.831971
56	8	0	-2.287700	-3.192202	2.609596
57	8	0	-0.863592	-1.623141	1.809025
58	7	0	-0.909117	1.691527	1.814872
59	7	0	0.897399	1.754110	-1.829523
60	1	0	-1.558995	1.139325	2.379050
61	1	0	1.563002	1.243697	-2.414967

E(RTPSSh) = -1516.46690938

Zero-point correction= 0.503314 (Hartree/Particle)

Thermal correction to Energy= 0.532241

Thermal correction to Enthalpy= 0.533186

Thermal correction to Gibbs Free Energy= 0.445547

Sum of electronic and zero-point Energies= -1515.963823

Sum of electronic and thermal Energies= -1515.934895

Sum of electronic and thermal Enthalpies= -1515.933951

Sum of electronic and thermal Free Energies= -1516.021590

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	0.000000	0.273832	0.000000
2	7	0	-1.627392	-1.424346	-1.521776
3	6	0	-2.227034	-2.519406	-0.698954
4	6	0	-2.550446	-2.156236	0.755796
5	6	0	-0.515639	-2.638732	2.112127
6	6	0	0.794650	-2.020615	2.611863
7	7	0	1.627392	-1.424346	1.521776
8	6	0	2.227034	-2.519406	0.698954
9	6	0	2.550446	-2.156236	-0.755796
10	6	0	0.515639	-2.638732	-2.112127
11	6	0	-0.794650	-2.020615	-2.611863
12	6	0	-2.685552	-0.564656	-2.137886
13	6	0	2.685552	-0.564656	2.137886
14	1	0	-1.513865	-3.347612	-0.692135
15	1	0	-3.139284	-2.897056	-1.185615
16	1	0	-3.337218	-1.403033	0.802794
17	1	0	-2.939332	-3.060343	1.247809
18	1	0	-0.328514	-3.433400	1.382815
19	1	0	-1.021582	-3.111344	2.967115
20	1	0	0.555094	-1.215642	3.315874
21	1	0	1.364564	-2.780865	3.168089
22	1	0	1.513865	-3.347612	0.692135
23	1	0	3.139284	-2.897056	1.185615
24	1	0	3.337218	-1.403033	-0.802794
25	1	0	2.939332	-3.060343	-1.247809

26	1	0	0.328514	-3.433400	-1.382815
27	1	0	1.021582	-3.111344	-2.967115
28	1	0	-0.555094	-1.215643	-3.315874
29	1	0	-1.364564	-2.780866	-3.168089
30	1	0	-2.195196	0.052168	-2.901908
31	1	0	-3.435325	-1.182951	-2.654297
32	1	0	2.195196	0.052168	2.901908
33	1	0	3.435325	-1.182951	2.654297
34	6	0	-3.361975	0.357489	-1.139205
35	6	0	-4.708298	0.717132	-1.219531
36	6	0	-5.222828	1.608235	-0.268896
37	1	0	-5.341103	0.313584	-2.004011
38	6	0	-3.064988	1.666102	0.776115
39	6	0	-4.397251	2.084299	0.750446
40	1	0	-6.265002	1.909271	-0.317641
41	1	0	-4.748829	2.752169	1.528816
42	6	0	3.361975	0.357489	1.139205
43	6	0	4.708298	0.717132	1.219531
44	6	0	3.064988	1.666102	-0.776115
45	6	0	5.222828	1.608235	0.268896
46	1	0	5.341103	0.313584	2.004011
47	6	0	4.397251	2.084299	-0.750446
48	1	0	6.265002	1.909271	0.317641
49	1	0	4.748829	2.752169	-1.528816
50	7	0	2.566635	0.843898	0.168219
51	7	0	-2.566635	0.843898	-0.168219
52	6	0	-2.115915	2.058611	1.912491
53	8	0	-0.921687	1.523773	1.809949
54	8	0	-2.538672	2.778403	2.805122
55	6	0	2.115915	2.058611	-1.912491
56	8	0	2.538672	2.778402	-2.805122
57	8	0	0.921687	1.523773	-1.809949
58	7	0	1.365893	-1.619352	-1.465803
59	7	0	-1.365893	-1.619352	1.465803
60	1	0	-1.689643	-0.971310	2.188041
61	1	0	1.689643	-0.971310	-2.188041

E(RTPSSh) = -1516.45913158

Zero-point correction= 0.503888 (Hartree/Particle)

Thermal correction to Energy= 0.532768

Thermal correction to Enthalpy= 0.533712

Thermal correction to Gibbs Free Energy= 0.446275

Sum of electronic and zero-point Energies= -1515.961940

Sum of electronic and thermal Energies= -1515.933060

Sum of electronic and thermal Enthalpies= -1515.932116

Sum of electronic and thermal Free Energies= -1516.019553

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	0.000000	0.198425	0.000000
2	7	0	1.733615	-1.191311	-1.596732
3	6	0	0.905357	-1.757972	-2.699526
4	6	0	-0.248539	-2.653342	-2.233648
5	6	0	-1.805818	-2.916321	-0.316311
6	6	0	-2.527335	-2.202377	0.836839
7	7	0	-1.733615	-1.191311	1.596733
8	6	0	-0.905356	-1.757971	2.699526
9	6	0	0.248539	-2.653342	2.233648
10	6	0	1.805819	-2.916321	0.316311
11	6	0	2.527336	-2.202377	-0.836838
12	6	0	2.675837	-0.180907	-2.175728
13	6	0	-2.675836	-0.180907	2.175728
14	1	0	1.531437	-2.332779	-3.401067
15	1	0	0.491592	-0.903526	-3.246424
16	1	0	-1.053990	-3.611183	0.060910
17	1	0	-2.555563	-3.524755	-0.844496
18	1	0	-3.386259	-1.670676	0.416213
19	1	0	-2.930094	-2.964520	1.522074
20	1	0	-1.531436	-2.332779	3.401068

21	1	0	-0.491592	-0.903526	3.246424
22	1	0	1.053991	-3.611183	-0.060910
23	1	0	2.555564	-3.524754	0.844497
24	1	0	3.386259	-1.670676	-0.416213
25	1	0	2.930094	-2.964519	-1.522074
26	1	0	3.445893	-0.666318	-2.793533
27	1	0	2.089449	0.470609	-2.835662
28	1	0	-3.445893	-0.666318	2.793534
29	1	0	-2.089449	0.470609	2.835662
30	6	0	3.318917	0.659172	-1.084220
31	6	0	4.620593	1.159281	-1.142950
32	6	0	5.085976	1.941548	-0.077187
33	1	0	5.257210	0.945664	-1.995917
34	6	0	2.972074	1.643020	1.013284
35	6	0	4.260172	2.182118	1.022394
36	1	0	6.093682	2.345226	-0.103964
37	1	0	4.579478	2.761474	1.881440
38	6	0	-3.318917	0.659172	1.084220
39	6	0	-4.620593	1.159281	1.142950
40	6	0	-2.972075	1.643020	-1.013284
41	6	0	-5.085977	1.941548	0.077187
42	1	0	-5.257210	0.945664	1.995918
43	6	0	-4.260172	2.182117	-1.022394
44	1	0	-6.093683	2.345226	0.103963
45	1	0	-4.579479	2.761473	-1.881440
46	7	0	-2.525108	0.915138	0.027589
47	7	0	2.525108	0.915138	-0.027589
48	6	0	2.003741	1.805510	2.188455
49	8	0	0.830792	1.252680	1.985014
50	8	0	2.389245	2.392417	3.189242
51	6	0	-2.003741	1.805510	-2.188455
52	8	0	-2.389246	2.392417	-3.189242
53	8	0	-0.830793	1.252680	-1.985014
54	1	0	0.824689	-2.950082	3.119868
55	1	0	-0.132115	-3.577278	1.792452
56	1	0	0.132115	-3.577278	-1.792452

57	1	0	-0.824688	-2.950083	-3.119868
58	7	0	1.110918	-1.978955	1.225143
59	7	0	-1.110918	-1.978955	-1.225143
60	1	0	1.812491	-1.430229	1.730774
61	1	0	-1.812491	-1.430230	-1.730774

E(RTPSSh) = -1516.45511723

Zero-point correction= 0.504311 (Hartree/Particle)

Thermal correction to Energy= 0.533083

Thermal correction to Enthalpy= 0.534027

Thermal correction to Gibbs Free Energy= 0.447331

Sum of electronic and zero-point Energies= -1515.957542

Sum of electronic and thermal Energies= -1515.928771

Sum of electronic and thermal Enthalpies= -1515.927826

Sum of electronic and thermal Free Energies= -1516.014523

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.592740	-1.798633	-1.036112
2	6	0	0.817572	-2.654098	-1.992317
3	6	0	-0.232788	-1.886791	-2.800219
4	6	0	-2.359861	-1.954060	-1.428928
5	6	0	-2.108670	-2.653167	-0.082568
6	7	0	-1.592740	-1.798633	1.036112
7	6	0	-0.817572	-2.654098	1.992317
8	6	0	0.232788	-1.886791	2.800219
9	6	0	2.359861	-1.954060	1.428928
10	6	0	2.108670	-2.653167	0.082568
11	6	0	2.714317	-1.159572	-1.791175
12	6	0	-2.714317	-1.159572	1.791175
13	1	0	0.316519	-3.430187	-1.410191
14	1	0	1.496198	-3.173139	-2.686359
15	1	0	-3.201031	-1.264297	-1.344481

16	1	0	-2.657549	-2.737611	-2.142948
17	1	0	-3.043304	-3.149297	0.221725
18	1	0	-1.375841	-3.448716	-0.235415
19	1	0	-0.316519	-3.430187	1.410191
20	1	0	-1.496198	-3.173139	2.686359
21	1	0	3.201031	-1.264297	1.344481
22	1	0	2.657549	-2.737611	2.142948
23	1	0	3.043304	-3.149297	-0.221725
24	1	0	1.375841	-3.448716	0.235415
25	1	0	3.452333	-1.921778	-2.085287
26	1	0	2.292353	-0.754586	-2.719861
27	1	0	-3.452333	-1.921778	2.085287
28	1	0	-2.292353	-0.754586	2.719861
29	6	0	3.400632	-0.033979	-1.041797
30	6	0	4.762286	0.242278	-1.176362
31	6	0	5.298124	1.331034	-0.477066
32	1	0	5.390208	-0.374655	-1.811943
33	6	0	3.129521	1.727205	0.468760
34	6	0	4.476483	2.080728	0.365045
35	1	0	6.352094	1.572818	-0.575956
36	1	0	4.841429	2.913295	0.955980
37	6	0	-3.400632	-0.033979	1.041797
38	6	0	-4.762286	0.242278	1.176362
39	6	0	-3.129521	1.727205	-0.468760
40	6	0	-5.298124	1.331034	0.477066
41	1	0	-5.390208	-0.374655	1.811943
42	6	0	-4.476483	2.080728	-0.365045
43	1	0	-6.352094	1.572818	0.575956
44	1	0	-4.841429	2.913295	-0.955980
45	7	0	-2.608321	0.711164	0.249396
46	7	0	2.608321	0.711164	-0.249396
47	6	0	2.191328	2.414893	1.464405
48	8	0	0.995304	1.880764	1.503527
49	8	0	2.629303	3.332655	2.141982
50	6	0	-2.191328	2.414893	-1.464405
51	8	0	-2.629303	3.332655	-2.141982

52	8	0	-0.995304	1.880764	-1.503527
53	1	0	0.727059	-2.599630	3.478090
54	1	0	-0.246335	-1.130686	3.432055
55	1	0	0.246335	-1.130686	-3.432055
56	1	0	-0.727059	-2.599630	-3.478090
57	7	0	1.208217	-1.175980	1.944941
58	7	0	-1.208217	-1.175981	-1.944941
59	57	0	0.000000	0.326337	0.000000
60	1	0	-1.580513	-0.392162	-2.483065
61	1	0	1.580513	-0.392162	2.483065

E(RTPSSh) = -1516.44695576

Zero-point correction= 0.504507 (Hartree/Particle)

Thermal correction to Energy= 0.533269

Thermal correction to Enthalpy= 0.534213

Thermal correction to Gibbs Free Energy= 0.446781

Sum of electronic and zero-point Energies= -1515.950549

Sum of electronic and thermal Energies= -1515.921786

Sum of electronic and thermal Enthalpies= -1515.920842

Sum of electronic and thermal Free Energies= -1516.008274

[Nd(dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	0.000000	0.080585	0.000000
2	7	0	-1.928212	-1.595107	1.082306
3	6	0	-1.342353	-2.584447	2.032312
4	6	0	-0.071871	-2.083779	2.723834

5	6	0	1.696030	-2.829189	1.108549
6	6	0	2.640385	-2.305227	0.022506
7	7	0	1.928213	-1.595107	-1.082306
8	6	0	1.342353	-2.584447	-2.032312
9	6	0	0.071871	-2.083779	-2.723834
10	6	0	-1.696030	-2.829189	-1.108549
11	6	0	-2.640385	-2.305227	-0.022506
12	6	0	-2.879318	-0.691225	1.797388
13	6	0	2.879318	-0.691225	-1.797388
14	1	0	-1.113676	-3.492467	1.466341
15	1	0	-2.080871	-2.872399	2.794777
16	1	0	-0.282539	-1.185549	3.313381
17	1	0	0.276814	-2.859763	3.421604
18	1	0	0.958147	-3.515215	0.679067
19	1	0	2.281848	-3.409218	1.837401
20	1	0	3.338481	-1.596476	0.477440
21	1	0	3.238187	-3.137616	-0.378269
22	1	0	1.113676	-3.492467	-1.466340
23	1	0	2.080871	-2.872399	-2.794777
24	1	0	0.282539	-1.185549	-3.313380
25	1	0	-0.276814	-2.859763	-3.421604
26	1	0	-0.958147	-3.515215	-0.679067
27	1	0	-2.281848	-3.409218	-1.837401
28	1	0	-3.338481	-1.596476	-0.477440
29	1	0	-3.238187	-3.137616	0.378270
30	1	0	-3.746055	-1.256166	2.173116
31	1	0	-2.355982	-0.281652	2.670541
32	1	0	3.746055	-1.256166	-2.173116
33	1	0	2.355982	-0.281652	-2.670541
34	6	0	-3.341452	0.448631	0.905126
35	6	0	-4.595959	1.051505	1.004219
36	6	0	-4.905806	2.099770	0.128058
37	1	0	-5.315026	0.713819	1.744160
38	6	0	-2.748579	1.838241	-0.883246
39	6	0	-3.979492	2.494786	-0.838905
40	1	0	-5.873036	2.589011	0.192755

41	1	0	-4.179832	3.281385	-1.557587
42	6	0	3.341452	0.448631	-0.905126
43	6	0	4.595959	1.051505	-1.004219
44	6	0	2.748578	1.838241	0.883246
45	6	0	4.905806	2.099770	-0.128058
46	1	0	5.315026	0.713818	-1.744160
47	6	0	3.979492	2.494786	0.838905
48	1	0	5.873036	2.589010	-0.192756
49	1	0	4.179832	3.281385	1.557587
50	7	0	2.446515	0.854835	0.013370
51	7	0	-2.446515	0.854835	-0.013370
52	6	0	-1.683796	2.149675	-1.937348
53	8	0	-0.586834	1.440860	-1.794569
54	8	0	-1.933634	2.975931	-2.801639
55	6	0	1.683796	2.149675	1.937348
56	8	0	1.933634	2.975931	2.801639
57	8	0	0.586834	1.440861	1.794569
58	7	0	0.973832	-1.709095	1.742959
59	7	0	-0.973832	-1.709096	-1.742959
60	1	0	1.652454	-1.116437	2.226989
61	1	0	-1.652454	-1.116437	-2.226988

E(RTPSSh) = -1518.36535530

Zero-point correction= 0.504696 (Hartree/Particle)

Thermal correction to Energy= 0.533312

Thermal correction to Enthalpy= 0.534256

Thermal correction to Gibbs Free Energy= 0.447466

Sum of electronic and zero-point Energies= -1517.867852

Sum of electronic and thermal Energies= -1517.839235

Sum of electronic and thermal Enthalpies= -1517.838291

Sum of electronic and thermal Free Energies= -1517.925082

F2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	60	0	0.000000	0.184739	0.000000
2	7	0	-1.624407	-1.422874	-1.509669
3	6	0	-2.234402	-2.517123	-0.693359
4	6	0	-2.547192	-2.154273	0.763485
5	6	0	-0.505828	-2.644066	2.114252
6	6	0	0.803823	-2.020198	2.608308
7	7	0	1.624407	-1.422874	1.509669
8	6	0	2.234402	-2.517123	0.693359
9	6	0	2.547192	-2.154274	-0.763486
10	6	0	0.505827	-2.644066	-2.114252
11	6	0	-0.803823	-2.020199	-2.608308
12	6	0	-2.672319	-0.538542	-2.108156
13	6	0	2.672319	-0.538542	2.108156
14	1	0	-1.529697	-3.352739	-0.692622
15	1	0	-3.151941	-2.881486	-1.179832
16	1	0	-3.327724	-1.394639	0.815517
17	1	0	-2.938592	-3.054750	1.259509
18	1	0	-0.319784	-3.443396	1.389515
19	1	0	-1.013131	-3.109759	2.972048
20	1	0	0.563473	-1.213622	3.309673
21	1	0	1.381201	-2.775825	3.162683
22	1	0	1.529696	-3.352739	0.692623
23	1	0	3.151941	-2.881486	1.179832
24	1	0	3.327724	-1.394640	-0.815517
25	1	0	2.938591	-3.054751	-1.259508
26	1	0	0.319784	-3.443396	-1.389513
27	1	0	1.013131	-3.109760	-2.972048
28	1	0	-0.563473	-1.213624	-3.309673
29	1	0	-1.381201	-2.775827	-3.162683
30	1	0	-2.180584	0.065785	-2.880685
31	1	0	-3.447770	-1.138272	-2.607906
32	1	0	2.180584	0.065786	2.880685
33	1	0	3.447770	-1.138271	2.607906
34	6	0	-3.301179	0.404104	-1.097747
35	6	0	-4.629746	0.827453	-1.162494

36	6	0	-5.091287	1.738288	-0.203543
37	1	0	-5.289307	0.458257	-1.941760
38	6	0	-2.923007	1.693276	0.818102
39	6	0	-4.233577	2.174221	0.807889
40	1	0	-6.118717	2.087766	-0.240269
41	1	0	-4.545568	2.857427	1.589779
42	6	0	3.301179	0.404104	1.097747
43	6	0	4.629747	0.827453	1.162494
44	6	0	2.923007	1.693276	-0.818102
45	6	0	5.091287	1.738287	0.203542
46	1	0	5.289307	0.458258	1.941760
47	6	0	4.233577	2.174221	-0.807889
48	1	0	6.118717	2.087765	0.240268
49	1	0	4.545568	2.857427	-1.589779
50	7	0	2.476362	0.848703	0.132014
51	7	0	-2.476362	0.848703	-0.132013
52	6	0	-1.935296	2.036272	1.936199
53	8	0	-0.771321	1.440618	1.807587
54	8	0	-2.301126	2.773697	2.838917
55	6	0	1.935296	2.036273	-1.936199
56	8	0	2.301126	2.773698	-2.838918
57	8	0	0.771321	1.440618	-1.807586
58	7	0	1.352492	-1.624995	-1.462005
59	7	0	-1.352492	-1.624995	1.462005
60	1	0	-1.661074	-0.963745	2.178741
61	1	0	1.661074	-0.963745	-2.178742

E(RTPSSh) = -1518.36307226

Zero-point correction= 0.504948 (Hartree/Particle)

Thermal correction to Energy= 0.533412

Thermal correction to Enthalpy= 0.534356

Thermal correction to Gibbs Free Energy= 0.448195

Sum of electronic and zero-point Energies= -1517.865157

Sum of electronic and thermal Energies= -1517.836693

Sum of electronic and thermal Enthalpies= -1517.835748

Sum of electronic and thermal Free Energies= -1517.921910

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	0.000466	-0.178725	0.018481
2	7	0	1.691368	1.246377	1.543883
3	6	0	0.856574	1.873784	2.608932
4	6	0	-0.279173	2.739047	2.063100
5	6	0	-1.769287	2.899886	0.095402
6	6	0	-2.475788	2.129170	-1.022698
7	7	0	-1.672658	1.054312	-1.689744
8	6	0	-0.836688	1.544686	-2.822955
9	6	0	0.309715	2.456567	-2.387633
10	6	0	1.799514	2.851161	-0.457735
11	6	0	2.498958	2.227725	0.751864
12	6	0	2.638456	0.284452	2.180861
13	6	0	-2.622741	0.027234	-2.209441
14	1	0	1.479075	2.482655	3.281755
15	1	0	0.430372	1.052322	3.193158
16	1	0	-1.007706	3.568977	-0.304508
17	1	0	-2.520265	3.535483	0.584932
18	1	0	-3.355359	1.643388	-0.591729
19	1	0	-2.840525	2.844158	-1.773758
20	1	0	-1.456234	2.077486	-3.560030
21	1	0	-0.422441	0.656687	-3.310380
22	1	0	1.043110	3.573513	-0.150771
23	1	0	2.555560	3.411430	-1.025133
24	1	0	3.380149	1.690782	0.390577
25	1	0	2.860841	3.032154	1.407693
26	1	0	3.407733	0.808440	2.764349
27	1	0	2.063776	-0.336227	2.878653
28	1	0	-3.388123	0.481300	-2.853758
29	1	0	-2.049655	-0.674879	-2.826665
30	6	0	3.278121	-0.606146	1.132568

31	6	0	4.573030	-1.121745	1.236246
32	6	0	5.048997	-1.948212	0.213673
33	1	0	5.194125	-0.877212	2.091485
34	6	0	2.955713	-1.671579	-0.922277
35	6	0	4.234533	-2.227545	-0.886561
36	1	0	6.052132	-2.358947	0.271525
37	1	0	4.566115	-2.852094	-1.707751
38	6	0	-3.270815	-0.729008	-1.065120
39	6	0	-4.555227	-1.277129	-1.126542
40	6	0	-2.979286	-1.508503	1.117980
41	6	0	-5.040643	-1.972733	-0.015099
42	1	0	-5.160661	-1.157566	-2.018820
43	6	0	-4.247412	-2.088911	1.129236
44	1	0	-6.034832	-2.407850	-0.039607
45	1	0	-4.587778	-2.606652	2.018309
46	7	0	-2.512531	-0.854843	0.038074
47	7	0	2.500541	-0.887538	0.072138
48	6	0	1.991124	-1.894350	-2.082115
49	8	0	0.849537	-1.285426	-1.964531
50	8	0	2.351665	-2.609206	-3.024573
51	6	0	-2.040370	-1.553929	2.318212
52	8	0	-2.413163	-2.139298	3.342054
53	8	0	-0.906915	-0.944451	2.143554
54	1	0	0.926559	2.680752	-3.266041
55	1	0	-0.073023	3.412581	-2.025493
56	1	0	0.114423	3.638421	1.586134
57	1	0	-0.892769	3.076892	2.906772
58	7	0	1.125737	1.838508	-1.303722
59	7	0	-1.102162	2.000607	1.064055
60	1	0	1.849776	1.272904	-1.755466
61	1	0	-1.827199	1.496172	1.581513

E(RTPSSh) = -1518.36739458

Zero-point correction= 0.503934 (Hartree/Particle)

Thermal correction to Energy= 0.532888

Thermal correction to Enthalpy= 0.533832

Thermal correction to Gibbs Free Energy= 0.446283

Sum of electronic and zero-point Energies= -1517.863481

Sum of electronic and thermal Energies= -1517.834527

Sum of electronic and thermal Enthalpies= -1517.833583

Sum of electronic and thermal Free Energies= -1517.921132

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.523772	1.822725	-1.804152
2	6	0	-1.672730	1.373983	-2.656132
3	6	0	-2.742789	0.597915	-1.883745
4	6	0	-2.051434	-1.838183	-1.963443
5	6	0	-0.692174	-1.991654	-2.664283
6	7	0	0.523772	-1.822725	-1.804152
7	6	0	1.672730	-1.373983	-2.656132
8	6	0	2.742789	-0.597915	-1.883745
9	6	0	2.051434	1.838183	-1.963443
10	6	0	0.692174	1.991654	-2.664283
11	6	0	-0.905279	3.109084	-1.142492
12	6	0	0.905279	-3.109084	-1.142492
13	1	0	-1.269646	0.731899	-3.442214
14	1	0	-2.140713	2.232325	-3.161426
15	1	0	-2.215947	-2.667311	-1.273302
16	1	0	-2.825306	-1.910074	-2.742924
17	1	0	-0.670552	-2.973585	-3.161673
18	1	0	-0.623353	-1.243460	-3.457544
19	1	0	1.269646	-0.731899	-3.442214
20	1	0	2.140713	-2.232325	-3.161426
21	1	0	2.215947	2.667311	-1.273302
22	1	0	2.825306	1.910074	-2.742924
23	1	0	0.670552	2.973585	-3.161673
24	1	0	0.623353	1.243460	-3.457544
25	1	0	-0.944074	3.919079	-1.886914

26	1	0	-1.924809	2.985976	-0.755953
27	1	0	0.944074	-3.919079	-1.886914
28	1	0	1.924809	-2.985976	-0.755953
29	6	0	0.000000	3.499264	0.010608
30	6	0	0.265063	4.825899	0.354523
31	6	0	1.075530	5.080479	1.468227
32	1	0	-0.151032	5.641398	-0.229116
33	6	0	1.339813	2.714876	1.758759
34	6	0	1.629340	4.014421	2.178285
35	1	0	1.285806	6.104638	1.761427
36	1	0	2.287520	4.151780	3.028885
37	6	0	0.000000	-3.499264	0.010608
38	6	0	-0.265063	-4.825899	0.354523
39	6	0	-1.339813	-2.714876	1.758759
40	6	0	-1.075530	-5.080479	1.468227
41	1	0	0.151032	-5.641398	-0.229116
42	6	0	-1.629340	-4.014421	2.178285
43	1	0	-1.285806	-6.104638	1.761427
44	1	0	-2.287520	-4.151780	3.028885
45	7	0	-0.517830	-2.477651	0.715961
46	7	0	0.517830	2.477651	0.715961
47	6	0	1.998399	1.489371	2.397272
48	8	0	1.688732	0.364764	1.797473
49	8	0	2.759163	1.656097	3.338376
50	6	0	-1.998399	-1.489371	2.397272
51	8	0	-2.759163	-1.656097	3.338376
52	8	0	-1.688732	-0.364764	1.797473
53	1	0	3.541729	-0.322494	-2.588897
54	1	0	3.200919	-1.234015	-1.118483
55	1	0	-3.200919	1.234015	-1.118483
56	1	0	-3.541729	0.322494	-2.588897
57	7	0	2.194807	0.585467	-1.184579
58	7	0	-2.194807	-0.585467	-1.184579
59	60	0	0.000000	0.000000	0.236308
60	1	0	-2.797561	-0.779665	-0.383972
61	1	0	2.797561	0.779665	-0.383972

E(RTPSSh) = -1518.35254015

Zero-point correction= 0.503795 (Hartree/Particle)

Thermal correction to Energy= 0.532884

Thermal correction to Enthalpy= 0.533828

Thermal correction to Gibbs Free Energy= 0.445500

Sum of electronic and zero-point Energies= -1517.855356

Sum of electronic and thermal Energies= -1517.826268

Sum of electronic and thermal Enthalpies= -1517.825324

Sum of electronic and thermal Free Energies= -1517.913651

[Eu(dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000000	0.020260	0.000000
2	7	0	1.915875	-1.578536	-1.084141
3	6	0	1.336218	-2.560097	-2.046089
4	6	0	0.058146	-2.057151	-2.720897
5	6	0	-1.701637	-2.822395	-1.098778
6	6	0	-2.639536	-2.296687	-0.008170
7	7	0	-1.915875	-1.578536	1.084141
8	6	0	-1.336218	-2.560097	2.046089
9	6	0	-0.058146	-2.057151	2.720897
10	6	0	1.701637	-2.822394	1.098778
11	6	0	2.639536	-2.296687	0.008170
12	6	0	2.851893	-0.647294	-1.784302
13	6	0	-2.851893	-0.647294	1.784302
14	1	0	1.117920	-3.477666	-1.491074
15	1	0	2.073525	-2.830383	-2.815955
16	1	0	0.259392	-1.148722	-3.297335
17	1	0	-0.296050	-2.824841	-3.424649

18	1	0	-0.965327	-3.513845	-0.675002
19	1	0	-2.290973	-3.394442	-1.830845
20	1	0	-3.342938	-1.591503	-0.460906
21	1	0	-3.232354	-3.126852	0.403633
22	1	0	-1.117920	-3.477666	1.491074
23	1	0	-2.073525	-2.830383	2.815955
24	1	0	-0.259392	-1.148722	3.297335
25	1	0	0.296050	-2.824840	3.424650
26	1	0	0.965327	-3.513845	0.675002
27	1	0	2.290973	-3.394442	1.830845
28	1	0	3.342938	-1.591502	0.460906
29	1	0	3.232354	-3.126852	-0.403633
30	1	0	3.734352	-1.188446	-2.157870
31	1	0	2.325537	-0.238791	-2.655712
32	1	0	-3.734352	-1.188446	2.157871
33	1	0	-2.325537	-0.238791	2.655712
34	6	0	3.275570	0.493516	-0.874078
35	6	0	4.508180	1.142425	-0.956235
36	6	0	4.774051	2.189437	-0.064006
37	1	0	5.243505	0.841409	-1.695956
38	6	0	2.620065	1.841609	0.926124
39	6	0	3.827044	2.541310	0.899949
40	1	0	5.723841	2.713181	-0.115436
41	1	0	3.994223	3.327284	1.627758
42	6	0	-3.275570	0.493516	0.874078
43	6	0	-4.508180	1.142425	0.956235
44	6	0	-2.620065	1.841609	-0.926124
45	6	0	-4.774051	2.189437	0.064006
46	1	0	-5.243505	0.841409	1.695956
47	6	0	-3.827044	2.541310	-0.899949
48	1	0	-5.723841	2.713181	0.115436
49	1	0	-3.994223	3.327284	-1.627758
50	7	0	-2.362624	0.856395	-0.044251
51	7	0	2.362623	0.856395	0.044251
52	6	0	1.529113	2.103412	1.965942
53	8	0	0.458486	1.359705	1.794886

54	8	0	1.734851	2.925452	2.845471
55	6	0	-1.529113	2.103412	-1.965942
56	8	0	-1.734851	2.925452	-2.845471
57	8	0	-0.458486	1.359705	-1.794886
58	7	0	-0.978244	-1.697924	-1.723824
59	7	0	0.978244	-1.697924	1.723824
60	1	0	-1.657794	-1.093882	-2.191803
61	1	0	1.657794	-1.093882	2.191803

E(RTPSSh) = -1520.18520394

Zero-point correction= 0.504763 (Hartree/Particle)

Thermal correction to Energy= 0.533411

Thermal correction to Enthalpy= 0.534355

Thermal correction to Gibbs Free Energy= 0.447521

Sum of electronic and zero-point Energies= -1519.687587

Sum of electronic and thermal Energies= -1519.658939

Sum of electronic and thermal Enthalpies= -1519.657995

Sum of electronic and thermal Free Energies= -1519.744829

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000000	0.000000	0.110420
2	7	0	0.000000	2.206917	-1.418508
3	6	0	-1.015206	2.115794	-2.512316
4	6	0	-2.292579	1.348028	-2.151794
5	6	0	-1.890510	-1.069294	-2.646434
6	6	0	-1.362736	-2.362051	-2.015081
7	7	0	0.000000	-2.206917	-1.418508
8	6	0	1.015206	-2.115794	-2.512316
9	6	0	2.292579	-1.348028	-2.151794
10	6	0	1.890510	1.069294	-2.646434
11	6	0	1.362736	2.362051	-2.015081
12	6	0	-0.274629	3.362948	-0.509161

13	6	0	0.274629	-3.362948	-0.509161
14	1	0	-0.538731	1.609747	-3.356152
15	1	0	-1.283781	3.124161	-2.861574
16	1	0	-2.861319	1.878916	-1.387519
17	1	0	-2.925325	1.297526	-3.049893
18	1	0	-1.233889	-0.716854	-3.448746
19	1	0	-2.866590	-1.279530	-3.107723
20	1	0	-2.039233	-2.655812	-1.205382
21	1	0	-1.374509	-3.167965	-2.764420
22	1	0	0.538731	-1.609747	-3.356152
23	1	0	1.283781	-3.124161	-2.861574
24	1	0	2.861319	-1.878916	-1.387519
25	1	0	2.925325	-1.297526	-3.049893
26	1	0	1.233889	0.716854	-3.448746
27	1	0	2.866590	1.279530	-3.107723
28	1	0	2.039233	2.655812	-1.205382
29	1	0	1.374509	3.167965	-2.764420
30	1	0	0.631944	3.525034	0.086605
31	1	0	-0.456302	4.280059	-1.089024
32	1	0	-0.631944	-3.525034	0.086605
33	1	0	0.456302	-4.280059	-1.089024
34	6	0	-1.423464	3.100907	0.448067
35	6	0	-2.276434	4.096779	0.926944
36	6	0	-3.267602	3.743305	1.851609
37	1	0	-2.170763	5.123450	0.590408
38	6	0	-2.525341	1.468755	1.715096
39	6	0	-3.404165	2.411919	2.249802
40	1	0	-3.936530	4.503750	2.243217
41	1	0	-4.168556	2.081470	2.944015
42	6	0	1.423464	-3.100907	0.448067
43	6	0	2.276434	-4.096779	0.926944
44	6	0	2.525341	-1.468755	1.715096
45	6	0	3.267602	-3.743305	1.851609
46	1	0	2.170763	-5.123450	0.590408
47	6	0	3.404165	-2.411919	2.249802
48	1	0	3.936530	-4.503750	2.243217

49	1	0	4.168556	-2.081470	2.944015
50	7	0	1.552484	-1.825041	0.853881
51	7	0	-1.552484	1.825041	0.853881
52	6	0	-2.640751	-0.027798	2.012290
53	8	0	-1.756712	-0.757605	1.368228
54	8	0	-3.525621	-0.415632	2.759561
55	6	0	2.640751	0.027798	2.012290
56	8	0	3.525621	0.415632	2.759561
57	8	0	1.756712	0.757605	1.368228
58	7	0	1.981977	0.002963	-1.628191
59	7	0	-1.981977	-0.002963	-1.628191
60	1	0	-2.707915	-0.268926	-0.958753
61	1	0	2.707915	0.268926	-0.958753

E(RTPSSh) = -1520.18332384

Zero-point correction= 0.504564 (Hartree/Particle)

Thermal correction to Energy= 0.533311

Thermal correction to Enthalpy= 0.534255

Thermal correction to Gibbs Free Energy= 0.446875

Sum of electronic and zero-point Energies= -1519.685625

Sum of electronic and thermal Energies= -1519.656878

Sum of electronic and thermal Enthalpies= -1519.655933

Sum of electronic and thermal Free Energies= -1519.743313

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000000	0.045622	0.000000
2	7	0	1.722858	-1.180472	-1.558364
3	6	0	0.927848	-1.765308	-2.676275
4	6	0	-0.223312	-2.668176	-2.218982
5	6	0	-1.832953	-2.910676	-0.335803
6	6	0	-2.548143	-2.171506	0.805425
7	7	0	-1.722858	-1.180472	1.558364

8	6	0	-0.927848	-1.765308	2.676275
9	6	0	0.223312	-2.668177	2.218982
10	6	0	1.832953	-2.910676	0.335803
11	6	0	2.548143	-2.171506	-0.805425
12	6	0	2.620399	-0.114196	-2.107389
13	6	0	-2.620399	-0.114196	2.107389
14	1	0	1.575456	-2.336940	-3.360016
15	1	0	0.512397	-0.918332	-3.230862
16	1	0	-1.107665	-3.628501	0.051703
17	1	0	-2.589308	-3.493913	-0.881800
18	1	0	-3.387112	-1.616432	0.374429
19	1	0	-2.978103	-2.914617	1.494301
20	1	0	-1.575456	-2.336940	3.360016
21	1	0	-0.512397	-0.918332	3.230862
22	1	0	1.107665	-3.628501	-0.051703
23	1	0	2.589308	-3.493913	0.881800
24	1	0	3.387112	-1.616432	-0.374429
25	1	0	2.978103	-2.914617	-1.494301
26	1	0	3.431057	-0.547425	-2.711117
27	1	0	2.006807	0.513661	-2.764307
28	1	0	-3.431057	-0.547425	2.711117
29	1	0	-2.006807	0.513661	2.764307
30	6	0	3.178872	0.750638	-0.990915
31	6	0	4.433019	1.363097	-1.008773
32	6	0	4.798893	2.171881	0.075733
33	1	0	5.107709	1.216420	-1.846381
34	6	0	2.690774	1.685092	1.103729
35	6	0	3.924761	2.334329	1.153001
36	1	0	5.768103	2.661536	0.079488
37	1	0	4.168341	2.936810	2.020874
38	6	0	-3.178872	0.750638	0.990915
39	6	0	-4.433019	1.363097	1.008773
40	6	0	-2.690774	1.685092	-1.103729
41	6	0	-4.798893	2.171881	-0.075733
42	1	0	-5.107709	1.216420	1.846381
43	6	0	-3.924761	2.334329	-1.153001

44	1	0	-5.768103	2.661536	-0.079488
45	1	0	-4.168341	2.936810	-2.020874
46	7	0	-2.342101	0.925570	-0.048148
47	7	0	2.342101	0.925570	0.048148
48	6	0	1.662161	1.756777	2.233005
49	8	0	0.555561	1.094707	1.974380
50	8	0	1.938181	2.375371	3.249833
51	6	0	-1.662160	1.756777	-2.233005
52	8	0	-1.938181	2.375371	-3.249833
53	8	0	-0.555561	1.094707	-1.974380
54	1	0	0.791564	-2.974980	3.106793
55	1	0	-0.154834	-3.586064	1.763304
56	1	0	0.154834	-3.586064	-1.763304
57	1	0	-0.791564	-2.974980	-3.106793
58	7	0	1.095936	-1.985316	1.224209
59	7	0	-1.095936	-1.985316	-1.224209
60	1	0	1.773702	-1.419135	1.742879
61	1	0	-1.773702	-1.419135	-1.742880

E(RTPSSh) = -1520.18574651

Zero-point correction= 0.504556 (Hartree/Particle)

Thermal correction to Energy= 0.533401

Thermal correction to Enthalpy= 0.534345

Thermal correction to Gibbs Free Energy= 0.447068

Sum of electronic and zero-point Energies= -1519.683712

Sum of electronic and thermal Energies= -1519.654867

Sum of electronic and thermal Enthalpies= -1519.653923

Sum of electronic and thermal Free Energies= -1519.741200

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.088672	1.549016	-1.806613
2	6	0	-2.040278	0.758957	-2.653482

3	6	0	-2.785404	-0.327486	-1.874463
4	6	0	-1.333844	-2.403303	-1.971646
5	6	0	0.000000	-2.105201	-2.673122
6	7	0	1.088672	-1.549016	-1.806613
7	6	0	2.040278	-0.758957	-2.653482
8	6	0	2.785404	0.327486	-1.874463
9	6	0	1.333844	2.403303	-1.971646
10	6	0	0.000000	2.105201	-2.673122
11	6	0	-1.855168	2.638747	-1.125026
12	6	0	1.855168	-2.638747	-1.125026
13	1	0	-1.460111	0.288038	-3.450184
14	1	0	-2.768341	1.421938	-3.144363
15	1	0	-1.219613	-3.242707	-1.283540
16	1	0	-2.047101	-2.718302	-2.748131
17	1	0	0.343791	-3.024153	-3.172304
18	1	0	-0.178554	-1.372196	-3.463768
19	1	0	1.460111	-0.288038	-3.450184
20	1	0	2.768341	-1.421938	-3.144363
21	1	0	1.219613	3.242707	-1.283540
22	1	0	2.047101	2.718302	-2.748131
23	1	0	-0.343791	3.024153	-3.172304
24	1	0	0.178554	1.372196	-3.463768
25	1	0	-2.139613	3.413118	-1.853586
26	1	0	-2.787354	2.196134	-0.752661
27	1	0	2.139613	-3.413118	-1.853586
28	1	0	2.787354	-2.196134	-0.752661
29	6	0	-1.122073	3.261189	0.048545
30	6	0	-1.300206	4.587465	0.445719
31	6	0	-0.612465	5.046180	1.576515
32	1	0	-1.959600	5.246942	-0.110175
33	6	0	0.402431	2.884027	1.782239
34	6	0	0.257354	4.189614	2.253152
35	1	0	-0.743844	6.071154	1.910038
36	1	0	0.836107	4.499323	3.116114
37	6	0	1.122073	-3.261189	0.048545
38	6	0	1.300206	-4.587465	0.445719

39	6	0	-0.402431	-2.884027	1.782239
40	6	0	0.612465	-5.046180	1.576515
41	1	0	1.959600	-5.246942	-0.110175
42	6	0	-0.257354	-4.189614	2.253152
43	1	0	0.743844	-6.071154	1.910038
44	1	0	-0.836107	-4.499323	3.116114
45	7	0	0.298949	-2.437168	0.720424
46	7	0	-0.298949	2.437168	0.720424
47	6	0	1.417052	1.906525	2.379546
48	8	0	1.483341	0.769553	1.727191
49	8	0	2.084296	2.263941	3.337964
50	6	0	-1.417052	-1.906525	2.379546
51	8	0	-2.084296	-2.263941	3.337964
52	8	0	-1.483341	-0.769553	1.727191
53	1	0	3.457933	0.851529	-2.570100
54	1	0	3.415890	-0.120391	-1.098734
55	1	0	-3.415890	0.120391	-1.098734
56	1	0	-3.457933	-0.851529	-2.570100
57	7	0	1.865510	1.262857	-1.189047
58	7	0	-1.865510	-1.262857	-1.189047
59	63	0	0.000000	0.000000	0.167426
60	1	0	2.355012	1.635807	-0.374976
61	1	0	-2.355012	-1.635807	-0.374976

E(RTPSSh) = -1520.17265001 Zero-point correction= 0.504649 (Hartree/Particle)

Thermal correction to Energy= 0.533367

Thermal correction to Enthalpy= 0.534311

Thermal correction to Gibbs Free Energy= 0.447741

Sum of electronic and zero-point Energies= -1519.674133

Sum of electronic and thermal Energies= -1519.645415

Sum of electronic and thermal Enthalpies= -1519.644471

Sum of electronic and thermal Free Energies= -1519.731042

[Gd(dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.003657	0.000000
2	7	0	1.911012	-1.572496	-1.086444
3	6	0	1.332593	-2.551655	-2.051606
4	6	0	0.051238	-2.049036	-2.720223
5	6	0	-1.704667	-2.819674	-1.094124
6	6	0	-2.639375	-2.293154	-0.001139
7	7	0	-1.911012	-1.572496	1.086444
8	6	0	-1.332593	-2.551656	2.051606
9	6	0	-0.051238	-2.049037	2.720223
10	6	0	1.704666	-2.819675	1.094123
11	6	0	2.639375	-2.293155	0.001139
12	6	0	2.840982	-0.631972	-1.782500
13	6	0	-2.840982	-0.631972	1.782499
14	1	0	1.118451	-3.472217	-1.499806
15	1	0	2.068848	-2.816106	-2.824437
16	1	0	0.248651	-1.138052	-3.293758
17	1	0	-0.305051	-2.815026	-3.424630
18	1	0	-0.968434	-3.512794	-0.672862
19	1	0	-2.295986	-3.389276	-1.826398
20	1	0	-3.344876	-1.589104	-0.452528
21	1	0	-3.230210	-3.122563	0.414755
22	1	0	-1.118452	-3.472217	1.499805
23	1	0	-2.068849	-2.816107	2.824436
24	1	0	-0.248651	-1.138053	3.293758
25	1	0	0.305051	-2.815027	3.424630
26	1	0	0.968434	-3.512795	0.672861
27	1	0	2.295985	-3.389277	1.826397
28	1	0	3.344875	-1.589104	0.452527
29	1	0	3.230209	-3.122564	-0.414756
30	1	0	3.727258	-1.165194	-2.158227

31	1	0	2.311492	-0.222083	-2.651260
32	1	0	-3.727259	-1.165194	2.158227
33	1	0	-2.311493	-0.222083	2.651260
34	6	0	3.254827	0.507460	-0.865868
35	6	0	4.480896	1.169306	-0.942718
36	6	0	4.734627	2.214386	-0.044596
37	1	0	5.220326	0.879828	-1.682932
38	6	0	2.582290	1.841264	0.939322
39	6	0	3.782337	2.552789	0.919093
40	1	0	5.679257	2.747771	-0.091790
41	1	0	3.940398	3.337394	1.650417
42	6	0	-3.254827	0.507461	0.865868
43	6	0	-4.480896	1.169307	0.942718
44	6	0	-2.582289	1.841264	-0.939322
45	6	0	-4.734627	2.214387	0.044596
46	1	0	-5.220326	0.879829	1.682932
47	6	0	-3.782336	2.552790	-0.919093
48	1	0	-5.679256	2.747772	0.091790
49	1	0	-3.940397	3.337395	-1.650417
50	7	0	-2.337442	0.856929	-0.053045
51	7	0	2.337442	0.856929	0.053045
52	6	0	1.484037	2.088111	1.974931
53	8	0	0.419938	1.337179	1.794045
54	8	0	1.678316	2.906355	2.860622
55	6	0	-1.484036	2.088111	-1.974931
56	8	0	-1.678315	2.906355	-2.860622
57	8	0	-0.419938	1.337179	-1.794044
58	7	0	-0.981446	-1.694091	-1.717494
59	7	0	0.981446	-1.694091	1.717494
60	1	0	-1.661949	-1.087219	-2.180366
61	1	0	1.661948	-1.087220	2.180366

E(RTPSSh) = -1520.77552871

Zero-point correction= 0.504913 (Hartree/Particle)

Thermal correction to Energy= 0.533433

Thermal correction to Enthalpy= 0.534377

Thermal correction to Gibbs Free Energy= 0.447985

Sum of electronic and zero-point Energies= -1520.278483

Sum of electronic and thermal Energies= -1520.249963

Sum of electronic and thermal Enthalpies= -1520.249019

Sum of electronic and thermal Free Energies= -1520.335411

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.089115	0.000000
2	7	0	1.621897	-1.418403	1.492490
3	6	0	2.245748	-2.511704	0.685886
4	6	0	2.544593	-2.150899	-0.774055
5	6	0	0.493000	-2.647465	-2.115034
6	6	0	-0.815369	-2.015224	-2.601632
7	7	0	-1.621897	-1.418403	-1.492490
8	6	0	-2.245749	-2.511703	-0.685886
9	6	0	-2.544593	-2.150898	0.774055
10	6	0	-0.493000	-2.647464	2.115034
11	6	0	0.815369	-2.015224	2.601632
12	6	0	2.654948	-0.502769	2.069700
13	6	0	-2.654948	-0.502768	-2.069700
14	1	0	1.552982	-3.357444	0.694552
15	1	0	3.170490	-2.857633	1.171693
16	1	0	3.318951	-1.385104	-0.833232
17	1	0	2.936894	-3.047959	-1.274747
18	1	0	0.307696	-3.450514	-1.393983
19	1	0	1.000180	-3.107392	-2.975740
20	1	0	-0.573043	-1.205259	-3.297764
21	1	0	-1.401586	-2.763765	-3.155745
22	1	0	-1.552983	-3.357444	-0.694552
23	1	0	-3.170491	-2.857632	-1.171693
24	1	0	-3.318951	-1.385103	0.833232
25	1	0	-2.936895	-3.047959	1.274747

26	1	0	-0.307697	-3.450514	1.393983
27	1	0	-1.000180	-3.107392	2.975740
28	1	0	0.573043	-1.205259	3.297764
29	1	0	1.401586	-2.763765	3.155745
30	1	0	2.159652	0.089233	2.848855
31	1	0	3.459118	-1.077589	2.552522
32	1	0	-2.159651	0.089234	-2.848854
33	1	0	-3.459117	-1.077589	-2.552522
34	6	0	3.227618	0.460231	1.045270
35	6	0	4.531693	0.956406	1.089508
36	6	0	4.928591	1.886393	0.119977
37	1	0	5.221454	0.629235	1.861297
38	6	0	2.752387	1.722376	-0.869544
39	6	0	4.034294	2.273800	-0.880131
40	1	0	5.935969	2.291192	0.140843
41	1	0	4.298228	2.972278	-1.666186
42	6	0	-3.227618	0.460231	-1.045270
43	6	0	-4.531693	0.956407	-1.089508
44	6	0	-2.752387	1.722376	0.869544
45	6	0	-4.928591	1.886394	-0.119977
46	1	0	-5.221454	0.629236	-1.861297
47	6	0	-4.034293	2.273801	0.880131
48	1	0	-5.935968	2.291193	-0.140843
49	1	0	-4.298227	2.972278	1.666186
50	7	0	-2.369796	0.855019	-0.087704
51	7	0	2.369797	0.855019	0.087705
52	6	0	1.720909	2.006900	-1.963033
53	8	0	0.593458	1.349753	-1.800921
54	8	0	2.021063	2.757019	-2.879042
55	6	0	-1.720909	2.006900	1.963033
56	8	0	-2.021062	2.757018	2.879043
57	8	0	-0.593457	1.349753	1.800921
58	7	0	-1.338431	-1.628888	1.458802
59	7	0	1.338430	-1.628889	-1.458802
60	1	0	1.631939	-0.957511	-2.172235
61	1	0	-1.631938	-0.957511	2.172234

E(RTPSSh) = -1520.77425770

Zero-point correction= 0.505682 (Hartree/Particle)

Thermal correction to Energy= 0.533885

Thermal correction to Enthalpy= 0.534829

Thermal correction to Gibbs Free Energy= 0.449619

Sum of electronic and zero-point Energies= -1520.276042

Sum of electronic and thermal Energies= -1520.247839

Sum of electronic and thermal Enthalpies= -1520.246895

Sum of electronic and thermal Free Energies= -1520.332105

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.025801	0.000000
2	7	0	1.727414	-1.180500	-1.547835
3	6	0	0.941231	-1.769225	-2.669916
4	6	0	-0.211903	-2.671785	-2.217231
5	6	0	-1.836139	-2.909894	-0.345819
6	6	0	-2.554292	-2.167657	0.791486
7	7	0	-1.727414	-1.180500	1.547835
8	6	0	-0.941230	-1.769225	2.669916
9	6	0	0.211903	-2.671784	2.217232
10	6	0	1.836140	-2.909894	0.345819
11	6	0	2.554292	-2.167657	-0.791486
12	6	0	2.621820	-0.108999	-2.091538
13	6	0	-2.621820	-0.108999	2.091538
14	1	0	1.594125	-2.341891	-3.347650
15	1	0	0.528387	-0.924078	-3.228936
16	1	0	-1.116461	-3.631428	0.045449
17	1	0	-2.591558	-3.488926	-0.897415
18	1	0	-3.388358	-1.608542	0.356170
19	1	0	-2.991116	-2.908484	1.478424
20	1	0	-1.594124	-2.341891	3.347650

21	1	0	-0.528386	-0.924078	3.228936
22	1	0	1.116461	-3.631427	-0.045449
23	1	0	2.591558	-3.488926	0.897415
24	1	0	3.388358	-1.608542	-0.356170
25	1	0	2.991116	-2.908484	-1.478424
26	1	0	3.440452	-0.537498	-2.687745
27	1	0	2.008640	0.513917	-2.753244
28	1	0	-3.440452	-0.537498	2.687745
29	1	0	-2.008640	0.513917	2.753244
30	6	0	3.163658	0.761746	-0.971895
31	6	0	4.409969	1.390234	-0.982148
32	6	0	4.758306	2.205008	0.103528
33	1	0	5.091875	1.251415	-1.815229
34	6	0	2.649846	1.693067	1.117893
35	6	0	3.874804	2.358276	1.174570
36	1	0	5.721136	2.707013	0.112930
37	1	0	4.104577	2.965681	2.042768
38	6	0	-3.163658	0.761746	0.971895
39	6	0	-4.409969	1.390234	0.982148
40	6	0	-2.649846	1.693067	-1.117893
41	6	0	-4.758306	2.205008	-0.103528
42	1	0	-5.091875	1.251415	1.815229
43	6	0	-3.874804	2.358276	-1.174570
44	1	0	-5.721136	2.707011	-0.112930
45	1	0	-4.104578	2.965681	-2.042768
46	7	0	-2.318202	0.926928	-0.061569
47	7	0	2.318201	0.926928	0.061569
48	6	0	1.610740	1.753792	2.237570
49	8	0	0.515303	1.076684	1.969887
50	8	0	1.868288	2.377927	3.255829
51	6	0	-1.610741	1.753792	-2.237570
52	8	0	-1.868289	2.377927	-3.255829
53	8	0	-0.515304	1.076684	-1.969887
54	1	0	0.775820	-2.980647	3.107068
55	1	0	-0.163676	-3.588470	1.757068
56	1	0	0.163677	-3.588470	-1.757068

57	1	0	-0.775819	-2.980647	-3.107068
58	7	0	1.089409	-1.986469	1.228348
59	7	0	-1.089409	-1.986470	-1.228348
60	1	0	1.761488	-1.417671	1.751635
61	1	0	-1.761487	-1.417671	-1.751635

E(RTPSSh) = -1520.77692583

Zero-point correction= 0.504675 (Hartree/Particle)

Thermal correction to Energy= 0.533458

Thermal correction to Enthalpy= 0.534402

Thermal correction to Gibbs Free Energy= 0.447493

Sum of electronic and zero-point Energies= -1520.275021

Sum of electronic and thermal Energies= -1520.246239

Sum of electronic and thermal Enthalpies= -1520.245295

Sum of electronic and thermal Free Energies= -1520.332204

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.599131	-1.807199	1.012285
2	6	0	-0.859051	-2.652413	2.004558
3	6	0	0.191557	-1.871611	2.797416
4	6	0	2.334750	-1.974087	1.446908
5	6	0	2.101864	-2.675575	0.100379
6	7	0	1.599131	-1.807199	-1.012285
7	6	0	0.859051	-2.652413	-2.004557
8	6	0	-0.191557	-1.871612	-2.797415
9	6	0	-2.334750	-1.974088	-1.446908
10	6	0	-2.101863	-2.675575	-0.100379
11	6	0	-2.723853	-1.119414	1.720763
12	6	0	2.723853	-1.119414	-1.720762
13	1	0	-0.362267	-3.452483	1.451103
14	1	0	-1.557900	-3.138683	2.701400
15	1	0	3.179426	-1.286720	1.373963

16	1	0	2.612925	-2.749837	2.175935
17	1	0	3.035915	-3.175105	-0.199301
18	1	0	1.360202	-3.465559	0.242908
19	1	0	0.362267	-3.452483	-1.451102
20	1	0	1.557900	-3.138683	-2.701399
21	1	0	-3.179427	-1.286721	-1.373962
22	1	0	-2.612925	-2.749838	-2.175934
23	1	0	-3.035914	-3.175105	0.199301
24	1	0	-1.360202	-3.465559	-0.242907
25	1	0	-3.517361	-1.842925	1.961800
26	1	0	-2.329191	-0.751404	2.675863
27	1	0	3.517361	-1.842925	-1.961801
28	1	0	2.329190	-0.751404	-2.675862
29	6	0	-3.297143	0.060197	0.957731
30	6	0	-4.625691	0.473372	1.070662
31	6	0	-5.036472	1.608970	0.360896
32	1	0	-5.323357	-0.073950	1.697088
33	6	0	-2.824942	1.788854	-0.546420
34	6	0	-4.130333	2.275156	-0.465835
35	1	0	-6.062633	1.954695	0.441727
36	1	0	-4.401178	3.141470	-1.058882
37	6	0	3.297143	0.060197	-0.957732
38	6	0	4.625691	0.473373	-1.070662
39	6	0	2.824942	1.788854	0.546420
40	6	0	5.036471	1.608970	-0.360896
41	1	0	5.323357	-0.073949	-1.697088
42	6	0	4.130333	2.275156	0.465835
43	1	0	6.062633	1.954696	-0.441728
44	1	0	4.401178	3.141470	1.058882
45	7	0	2.426356	0.721820	-0.175758
46	7	0	-2.426356	0.721821	0.175758
47	6	0	-1.790006	2.373282	-1.510141
48	8	0	-0.659183	1.706803	-1.518994
49	8	0	-2.101026	3.335396	-2.195055
50	6	0	1.790006	2.373282	1.510141
51	8	0	2.101026	3.335395	2.195056

52	8	0	0.659183	1.706804	1.518994
53	1	0	-0.683312	-2.564536	-3.496456
54	1	0	0.284782	-1.092808	-3.402694
55	1	0	-0.284782	-1.092807	3.402695
56	1	0	0.683312	-2.564535	3.496457
57	7	0	-1.169222	-1.190322	-1.919106
58	7	0	1.169221	-1.190321	1.919106
59	1	0	-1.516359	-0.372558	-2.421201
60	1	0	1.516358	-0.372557	2.421201
61	64	0	0.000000	0.148198	0.000000

E(RTPSSh) = -1520.76411325

Zero-point correction= 0.505221 (Hartree/Particle)

Thermal correction to Energy= 0.533737

Thermal correction to Enthalpy= 0.534681

Thermal correction to Gibbs Free Energy= 0.448286

Sum of electronic and zero-point Energies= -1520.265265

Sum of electronic and thermal Energies= -1520.236748

Sum of electronic and thermal Enthalpies= -1520.235804

Sum of electronic and thermal Free Energies= -1520.322199

[Ho(dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000000	0.000000	0.043857
2	7	0	-1.006875	1.941947	1.553369
3	6	0	0.000000	2.452505	2.528179
4	6	0	1.438088	2.305753	2.028112
5	6	0	2.024299	-0.014113	2.810143
6	6	0	2.212130	-1.438068	2.279002
7	7	0	1.006875	-1.941947	1.553369

8	6	0	0.000000	-2.452505	2.528179
9	6	0	-1.438088	-2.305753	2.028112
10	6	0	-2.024299	0.014113	2.810143
11	6	0	-2.212130	1.438068	2.279002
12	6	0	-1.404295	3.011149	0.587096
13	6	0	1.404295	-3.011149	0.587096
14	1	0	-0.123215	1.885544	3.456368
15	1	0	-0.197676	3.505211	2.776600
16	1	0	1.586556	2.885243	1.112088
17	1	0	2.123777	2.702115	2.791087
18	1	0	1.181031	0.032069	3.507905
19	1	0	2.921734	0.282037	3.373043
20	1	0	3.050614	-1.442213	1.575934
21	1	0	2.477169	-2.114878	3.104242
22	1	0	0.123215	-1.885544	3.456368
23	1	0	0.197676	-3.505211	2.776600
24	1	0	-1.586556	-2.885243	1.112088
25	1	0	-2.123777	-2.702115	2.791087
26	1	0	-1.181031	-0.032069	3.507905
27	1	0	-2.921734	-0.282037	3.373043
28	1	0	-3.050614	1.442213	1.575934
29	1	0	-2.477169	2.114878	3.104242
30	1	0	-1.953491	3.816356	1.097629
31	1	0	-0.485624	3.445198	0.174580
32	1	0	1.953491	-3.816356	1.097629
33	1	0	0.485624	-3.445198	0.174580
34	6	0	-2.232359	2.433401	-0.548836
35	6	0	-3.211369	3.138109	-1.250397
36	6	0	-3.888094	2.487327	-2.290611
37	1	0	-3.441285	4.167940	-0.995506
38	6	0	-2.607902	0.513875	-1.840618
39	6	0	-3.595590	1.154595	-2.588631
40	1	0	-4.648900	3.019578	-2.853576
41	1	0	-4.105314	0.602435	-3.370136
42	6	0	2.232359	-2.433401	-0.548836
43	6	0	3.211369	-3.138109	-1.250397

44	6	0	2.607902	-0.513875	-1.840618
45	6	0	3.888094	-2.487327	-2.290611
46	1	0	3.441285	-4.167940	-0.995506
47	6	0	3.595590	-1.154595	-2.588631
48	1	0	4.648900	-3.019578	-2.853576
49	1	0	4.105314	-0.602435	-3.370136
50	7	0	1.948755	-1.156190	-0.857499
51	7	0	-1.948755	1.156190	-0.857499
52	6	0	-2.219157	-0.950714	-2.043094
53	8	0	-1.228595	-1.337127	-1.268060
54	8	0	-2.839108	-1.624134	-2.851547
55	6	0	2.219157	0.950714	-2.043094
56	8	0	2.839108	1.624134	-2.851547
57	8	0	1.228595	1.337127	-1.268060
58	7	0	1.747792	0.897252	1.682313
59	7	0	-1.747792	-0.897252	1.682313
60	1	0	2.564996	0.907154	1.068047
61	1	0	-2.564996	-0.907154	1.068047

E(RTPSSh) = -1522.53878326

Zero-point correction= 0.505058 (Hartree/Particle)

Thermal correction to Energy= 0.533534

Thermal correction to Enthalpy= 0.534479

Thermal correction to Gibbs Free Energy= 0.448989

Sum of electronic and zero-point Energies= -1522.039165

Sum of electronic and thermal Energies= -1522.010688

Sum of electronic and thermal Enthalpies= -1522.009744

Sum of electronic and thermal Free Energies= -1522.095233

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000000	0.029079	0.000000
2	7	0	-1.622723	-1.412767	-1.477226

3	6	0	-2.256728	-2.504571	-0.676902
4	6	0	-2.540874	-2.145650	0.785999
5	6	0	-0.479087	-2.648776	2.113995
6	6	0	0.828737	-2.010980	2.594409
7	7	0	1.622723	-1.412767	1.477226
8	6	0	2.256728	-2.504570	0.676902
9	6	0	2.540874	-2.145650	-0.785999
10	6	0	0.479087	-2.648776	-2.113995
11	6	0	-0.828737	-2.010980	-2.594409
12	6	0	-2.644373	-0.474672	-2.038720
13	6	0	2.644373	-0.474672	2.038720
14	1	0	-1.574472	-3.358889	-0.694808
15	1	0	-3.188338	-2.835027	-1.159990
16	1	0	-3.310189	-1.375170	0.852930
17	1	0	-2.932468	-3.040188	1.291194
18	1	0	-0.295041	-3.453675	1.394505
19	1	0	-0.985542	-3.105521	2.976648
20	1	0	0.586202	-1.200138	3.288951
21	1	0	1.422421	-2.755293	3.145872
22	1	0	1.574472	-3.358889	0.694809
23	1	0	3.188338	-2.835027	1.159991
24	1	0	3.310189	-1.375170	-0.852930
25	1	0	2.932468	-3.040188	-1.291193
26	1	0	0.295041	-3.453676	-1.394503
27	1	0	0.985542	-3.105522	-2.976647
28	1	0	-0.586202	-1.200139	-3.288951
29	1	0	-1.422421	-2.755294	-3.145872
30	1	0	-2.146828	0.108435	-2.822663
31	1	0	-3.468683	-1.030917	-2.508812
32	1	0	2.146828	0.108436	2.822663
33	1	0	3.468683	-1.030917	2.508812
34	6	0	-3.175901	0.501424	-1.004738
35	6	0	-4.459246	1.050238	-1.035451
36	6	0	-4.809338	1.991728	-0.058915
37	1	0	-5.168312	0.755085	-1.802615
38	6	0	-2.632798	1.739660	0.908899

39	6	0	-3.891072	2.341555	0.933609
40	1	0	-5.799887	2.436503	-0.069458
41	1	0	-4.119825	3.049310	1.722382
42	6	0	3.175901	0.501424	1.004738
43	6	0	4.459246	1.050238	1.035451
44	6	0	2.632798	1.739660	-0.908899
45	6	0	4.809338	1.991728	0.058915
46	1	0	5.168312	0.755085	1.802615
47	6	0	3.891072	2.341555	-0.933610
48	1	0	5.799887	2.436503	0.069457
49	1	0	4.119825	3.049310	-1.722383
50	7	0	2.296592	0.858062	0.052591
51	7	0	-2.296592	0.858062	-0.052591
52	6	0	-1.572850	1.980617	1.984020
53	8	0	-0.473297	1.282159	1.796823
54	8	0	-1.825419	2.736690	2.909176
55	6	0	1.572850	1.980616	-1.984020
56	8	0	1.825419	2.736689	-2.909177
57	8	0	0.473297	1.282158	-1.796823
58	7	0	1.324096	-1.629566	-1.457067
59	7	0	-1.324096	-1.629566	1.457067
60	1	0	-1.605645	-0.952992	2.170122
61	1	0	1.605645	-0.952992	-2.170122

E(RTPSSh) = -1522.53766559

Zero-point correction= 0.505283 (Hartree/Particle)

Thermal correction to Energy= 0.533766

Thermal correction to Enthalpy= 0.534710

Thermal correction to Gibbs Free Energy= 0.448303

Sum of electronic and zero-point Energies= -1522.036565

Sum of electronic and thermal Energies= -1522.008082

Sum of electronic and thermal Enthalpies= -1522.007138

Sum of electronic and thermal Free Energies= -1522.093544

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000000	0.029679	0.000000
2	7	0	1.746050	1.181707	1.508654
3	6	0	0.992241	1.782893	2.646018
4	6	0	-0.169520	2.682658	2.212304
5	6	0	-1.841523	2.907494	0.383350
6	6	0	-2.574376	2.156316	-0.737626
7	7	0	-1.746050	1.181707	-1.508654
8	6	0	-0.992241	1.782893	-2.646018
9	6	0	0.169520	2.682658	-2.212303
10	6	0	1.841523	2.907494	-0.383350
11	6	0	2.574376	2.156316	0.737626
12	6	0	2.635322	0.098260	2.035548
13	6	0	-2.635322	0.098261	-2.035548
14	1	0	1.663869	2.359696	3.301291
15	1	0	0.591275	0.943794	3.221640
16	1	0	-1.139721	3.638710	-0.022567
17	1	0	-2.589953	3.475368	0.955320
18	1	0	-3.389969	1.584142	-0.284583
19	1	0	-3.036422	2.889469	-1.416028
20	1	0	-1.663869	2.359696	-3.301290
21	1	0	-0.591275	0.943794	-3.221640
22	1	0	1.139720	3.638710	0.022568
23	1	0	2.589953	3.475369	-0.955320
24	1	0	3.389969	1.584142	0.284583
25	1	0	3.036422	2.889469	1.416028
26	1	0	3.479927	0.516173	2.602118
27	1	0	2.029545	-0.508214	2.718027
28	1	0	-3.479928	0.516173	-2.602118
29	1	0	-2.029546	-0.508214	-2.718027
30	6	0	3.122032	-0.792314	0.908070
31	6	0	4.343247	-1.468354	0.895489
32	6	0	4.636450	-2.303102	-0.190739
33	1	0	5.047509	-1.351084	1.713110

34	6	0	2.527152	-1.718360	-1.161307
35	6	0	3.723211	-2.431117	-1.240109
36	1	0	5.578938	-2.841733	-0.217204
37	1	0	3.908831	-3.054817	-2.107279
38	6	0	-3.122032	-0.792314	-0.908070
39	6	0	-4.343247	-1.468354	-0.895489
40	6	0	-2.527152	-1.718360	1.161307
41	6	0	-4.636450	-2.303102	0.190739
42	1	0	-5.047509	-1.351084	-1.713110
43	6	0	-3.723211	-2.431117	1.240109
44	1	0	-5.578938	-2.841733	0.217204
45	1	0	-3.908831	-3.054818	2.107279
46	7	0	-2.248825	-0.929917	0.105743
47	7	0	2.248825	-0.929917	-0.105743
48	6	0	1.455925	-1.748740	-2.248864
49	8	0	0.396397	-1.026395	-1.952069
50	8	0	1.654522	-2.389965	-3.269351
51	6	0	-1.455925	-1.748740	2.248864
52	8	0	-1.654522	-2.389965	3.269351
53	8	0	-0.396397	-1.026395	1.952069
54	1	0	0.717848	2.996204	-3.110170
55	1	0	-0.194696	3.596789	-1.738133
56	1	0	0.194696	3.596789	1.738134
57	1	0	-0.717849	2.996203	3.110170
58	7	0	1.063634	1.988725	-1.244299
59	7	0	-1.063634	1.988725	1.244299
60	1	0	1.717964	1.414714	-1.784128
61	1	0	-1.717964	1.414713	1.784128

E(RTPSSh) = -1522.54024080

Zero-point correction= 0.505074 (Hartree/Particle)

Thermal correction to Energy= 0.533734

Thermal correction to Enthalpy= 0.534678

Thermal correction to Gibbs Free Energy= 0.448191

Sum of electronic and zero-point Energies= -1522.037402

Sum of electronic and thermal Energies= -1522.008742

Sum of electronic and thermal Enthalpies= -1522.007798

Sum of electronic and thermal Free Energies= -1522.094284

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.524564	1.815476	-1.808821
2	6	0	-1.690551	1.393770	-2.650645
3	6	0	-2.735549	0.599063	-1.865161
4	6	0	-2.035953	-1.836242	-1.979069
5	6	0	-0.679728	-1.991648	-2.681771
6	7	0	0.524564	-1.815476	-1.808821
7	6	0	1.690551	-1.393770	-2.650645
8	6	0	2.735549	-0.599063	-1.865161
9	6	0	2.035953	1.836242	-1.979069
10	6	0	0.679728	1.991648	-2.681771
11	6	0	-0.881258	3.085822	-1.101420
12	6	0	0.881258	-3.085822	-1.101420
13	1	0	-1.304777	0.769701	-3.460209
14	1	0	-2.167558	2.264794	-3.123708
15	1	0	-2.203554	-2.667302	-1.291456
16	1	0	-2.817149	-1.894287	-2.751294
17	1	0	-0.650387	-2.973057	-3.179289
18	1	0	-0.608456	-1.239969	-3.472266
19	1	0	1.304777	-0.769701	-3.460209
20	1	0	2.167558	-2.264794	-3.123708
21	1	0	2.203554	2.667302	-1.291456
22	1	0	2.817149	1.894287	-2.751294
23	1	0	0.650387	2.973057	-3.179289
24	1	0	0.608456	1.239969	-3.472266
25	1	0	-0.870455	3.928723	-1.808625
26	1	0	-1.913881	2.980518	-0.747083
27	1	0	0.870455	-3.928723	-1.808625
28	1	0	1.913881	-2.980518	-0.747083

29	6	0	0.000000	3.385344	0.096935
30	6	0	0.253782	4.676701	0.562278
31	6	0	1.035240	4.831207	1.714397
32	1	0	-0.148550	5.540881	0.042695
33	6	0	1.291137	2.450260	1.810609
34	6	0	1.569219	3.707285	2.347493
35	1	0	1.237425	5.825883	2.100149
36	1	0	2.200982	3.771390	3.226277
37	6	0	0.000000	-3.385344	0.096935
38	6	0	-0.253782	-4.676701	0.562278
39	6	0	-1.291137	-2.450260	1.810609
40	6	0	-1.035240	-4.831207	1.714397
41	1	0	0.148550	-5.540881	0.042695
42	6	0	-1.569219	-3.707285	2.347493
43	1	0	-1.237425	-5.825883	2.100149
44	1	0	-2.200982	-3.771390	3.226277
45	7	0	-0.503567	-2.309397	0.724991
46	7	0	0.503567	2.309397	0.724991
47	6	0	1.913225	1.163257	2.354911
48	8	0	1.611920	0.103152	1.640045
49	8	0	2.642652	1.227510	3.332003
50	6	0	-1.913225	-1.163257	2.354911
51	8	0	-2.642652	-1.227510	3.332003
52	8	0	-1.611920	-0.103152	1.640045
53	1	0	3.549552	-0.319829	-2.550331
54	1	0	3.177789	-1.219466	-1.078393
55	1	0	-3.177789	1.219466	-1.078393
56	1	0	-3.549552	0.319829	-2.550331
57	7	0	2.150297	0.584349	-1.194672
58	7	0	-2.150297	-0.584349	-1.194672
59	1	0	2.712870	0.774627	-0.365190
60	1	0	-2.712870	-0.774627	-0.365190
61	67	0	0.000000	0.000000	0.088970

E(RTPSSh) = -1522.52539000

Zero-point correction= 0.505230 (Hartree/Particle)

Thermal correction to Energy= 0.533664

Thermal correction to Enthalpy= 0.534609

Thermal correction to Gibbs Free Energy= 0.449447

Sum of electronic and zero-point Energies= -1522.025683

Sum of electronic and thermal Energies= -1521.997249

Sum of electronic and thermal Enthalpies= -1521.996304

Sum of electronic and thermal Free Energies= -1522.081466

[Yb(dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	0.000000	0.079250	0.000000
2	7	0	-1.887174	1.534886	-1.086159
3	6	0	-1.326401	2.507478	-2.067839
4	6	0	-0.032950	2.010941	-2.714533
5	6	0	1.712557	2.798312	-1.078045
6	6	0	2.637489	2.262863	0.018297
7	7	0	1.887173	1.534887	1.086159
8	6	0	1.326400	2.507478	2.067839
9	6	0	0.032949	2.010941	2.714533
10	6	0	-1.712558	2.798311	1.078045
11	6	0	-2.637490	2.262862	-0.018297
12	6	0	-2.785523	0.547840	-1.759853
13	6	0	2.785523	0.547841	1.759853
14	1	0	-1.131155	3.441157	-1.530665
15	1	0	-2.063904	2.743252	-2.848354
16	1	0	-0.215450	1.092758	-3.280102
17	1	0	0.333904	2.773455	-3.416588
18	1	0	0.981778	3.500669	-0.662191
19	1	0	2.308415	3.354632	-1.816261
20	1	0	3.344723	1.559593	-0.431983

21	1	0	3.226834	3.084215	0.450558
22	1	0	1.131154	3.441157	1.530665
23	1	0	2.063903	2.743253	2.848354
24	1	0	0.215449	1.092758	3.280102
25	1	0	-0.333905	2.773455	3.416588
26	1	0	-0.981780	3.500669	0.662191
27	1	0	-2.308416	3.354630	1.816261
28	1	0	-3.344724	1.559591	0.431983
29	1	0	-3.226835	3.084214	-0.450557
30	1	0	-3.691527	1.039461	-2.144203
31	1	0	-2.239886	0.131453	-2.614846
32	1	0	3.691527	1.039463	2.144202
33	1	0	2.239887	0.131454	2.614846
34	6	0	-3.144825	-0.582865	-0.810544
35	6	0	-4.331407	-1.315574	-0.859369
36	6	0	-4.517629	-2.349893	0.067496
37	1	0	-5.091341	-1.089422	-1.600768
38	6	0	-2.379491	-1.838002	1.015503
39	6	0	-3.537676	-2.614603	1.027009
40	1	0	-5.431370	-2.936004	0.043083
41	1	0	-3.643507	-3.392463	1.774795
42	6	0	3.144825	-0.582864	0.810544
43	6	0	4.331408	-1.315572	0.859369
44	6	0	2.379492	-1.838002	-1.015502
45	6	0	4.517631	-2.349890	-0.067497
46	1	0	5.091342	-1.089419	1.600767
47	6	0	3.537678	-2.614602	-1.027009
48	1	0	5.431373	-2.936002	-0.043084
49	1	0	3.643509	-3.392462	-1.774795
50	7	0	2.204812	-0.857343	-0.109682
51	7	0	-2.204812	-0.857343	0.109682
52	6	0	-1.240876	-2.003423	2.020831
53	8	0	-0.218357	-1.210292	1.779978
54	8	0	-1.363814	-2.801251	2.937237
55	6	0	1.240877	-2.003424	-2.020830
56	8	0	1.363815	-2.801252	-2.937235

57	8	0	0.218359	-1.210292	-1.779978
58	7	0	0.981704	1.669548	-1.687588
59	7	0	-0.981705	1.669548	1.687588
60	1	0	1.662460	1.047745	-2.129307
61	1	0	-1.662460	1.047744	2.129307

E(RTPSSh) = -1524.28870841

Zero-point correction= 0.504493 (Hartree/Particle)

Thermal correction to Energy= 0.533077

Thermal correction to Enthalpy= 0.534021

Thermal correction to Gibbs Free Energy= 0.447600

Sum of electronic and zero-point Energies= -1523.788015

Sum of electronic and thermal Energies= -1523.759431

Sum of electronic and thermal Enthalpies= -1523.758487

Sum of electronic and thermal Free Energies= -1523.844909

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	0.000000	0.019753	0.000000
2	7	0	-1.622455	1.402375	1.465851
3	6	0	-2.265842	2.494360	0.673839
4	6	0	-2.536230	2.140187	-0.792493
5	6	0	-0.467275	2.644816	-2.115209
6	6	0	0.837974	1.998344	-2.590772
7	7	0	1.622455	1.402375	-1.465851
8	6	0	2.265842	2.494360	-0.673839
9	6	0	2.536230	2.140187	0.792493
10	6	0	0.467275	2.644816	2.115209
11	6	0	-0.837975	1.998344	2.590772
12	6	0	-2.632686	0.443112	2.012050
13	6	0	2.632686	0.443112	-2.012050
14	1	0	-1.593502	3.356385	0.702096
15	1	0	-3.203704	2.809510	1.154715

16	1	0	-3.302149	1.366902	-0.867991
17	1	0	-2.925049	3.033795	-1.300791
18	1	0	-0.281892	3.454138	-1.400911
19	1	0	-0.974982	3.095285	-2.980199
20	1	0	0.592009	1.183733	-3.279435
21	1	0	1.438012	2.735622	-3.144415
22	1	0	1.593502	3.356385	-0.702096
23	1	0	3.203704	2.809510	-1.154715
24	1	0	3.302149	1.366902	0.867991
25	1	0	2.925049	3.033796	1.300791
26	1	0	0.281891	3.454139	1.400910
27	1	0	0.974982	3.095285	2.980199
28	1	0	-0.592009	1.183733	3.279435
29	1	0	-1.438013	2.735622	3.144415
30	1	0	-2.131302	-0.134936	2.796809
31	1	0	-3.473437	0.980966	2.473934
32	1	0	2.131302	-0.134936	-2.796810
33	1	0	3.473437	0.980966	-2.473934
34	6	0	-3.128538	-0.540606	0.967870
35	6	0	-4.390913	-1.136937	0.986937
36	6	0	-4.699509	-2.084787	0.002530
37	1	0	-5.114957	-0.873638	1.751695
38	6	0	-2.527379	-1.749524	-0.947654
39	6	0	-3.762158	-2.396687	-0.985105
40	1	0	-5.673074	-2.565705	0.004172
41	1	0	-3.959431	-3.109693	-1.777654
42	6	0	3.128538	-0.540606	-0.967870
43	6	0	4.390913	-1.136937	-0.986938
44	6	0	2.527379	-1.749524	0.947654
45	6	0	4.699510	-2.084787	-0.002530
46	1	0	5.114957	-0.873637	-1.751695
47	6	0	3.762158	-2.396687	0.985104
48	1	0	5.673075	-2.565705	-0.004172
49	1	0	3.959431	-3.109693	1.777655
50	7	0	2.232332	-0.859080	-0.018936
51	7	0	-2.232331	-0.859080	0.018936

52	6	0	-1.443883	-1.947808	-2.006505
53	8	0	-0.370261	-1.215791	-1.794108
54	8	0	-1.654044	-2.703462	-2.942528
55	6	0	1.443884	-1.947808	2.006505
56	8	0	1.654044	-2.703462	2.942528
57	8	0	0.370261	-1.215791	1.794108
58	7	0	1.310614	1.628178	1.451265
59	7	0	-1.310614	1.628178	-1.451265
60	1	0	-1.582052	0.943162	-2.160063
61	1	0	1.582052	0.943162	2.160063

E(RTPSSh) = -1524.28779964

Zero-point correction= 0.505095 (Hartree/Particle)

Thermal correction to Energy= 0.533575

Thermal correction to Enthalpy= 0.534519

Thermal correction to Gibbs Free Energy= 0.448449

Sum of electronic and zero-point Energies= -1523.786764

Sum of electronic and thermal Energies= -1523.758284

Sum of electronic and thermal Enthalpies= -1523.757340

Sum of electronic and thermal Free Energies= -1523.843410

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	0.000000	0.068492	0.000000
2	7	0	1.761855	1.180237	1.475309
3	6	0	1.036059	1.790392	2.625464
4	6	0	-0.134140	2.685690	2.208437
5	6	0	-1.843216	2.900348	0.416488
6	6	0	-2.589550	2.144640	-0.691140
7	7	0	-1.761855	1.180237	-1.475309
8	6	0	-1.036059	1.790392	-2.625464
9	6	0	0.134140	2.685691	-2.208436
10	6	0	1.843216	2.900348	-0.416489

11	6	0	2.589549	2.144641	0.691140
12	6	0	2.648938	0.088912	1.987653
13	6	0	-2.648938	0.088911	-1.987653
14	1	0	1.722534	2.371394	3.261030
15	1	0	0.647007	0.955827	3.215004
16	1	0	-1.155229	3.638316	-0.000919
17	1	0	-2.583612	3.459746	1.006576
18	1	0	-3.390266	1.562691	-0.224066
19	1	0	-3.071283	2.872842	-1.360925
20	1	0	-1.722535	2.371394	-3.261030
21	1	0	-0.647007	0.955826	-3.215004
22	1	0	1.155228	3.638316	0.000918
23	1	0	2.583611	3.459747	-1.006577
24	1	0	3.390266	1.562692	0.224066
25	1	0	3.071283	2.872842	1.360924
26	1	0	3.514793	0.499382	2.526730
27	1	0	2.052892	-0.504828	2.688879
28	1	0	-3.514792	0.499381	-2.526730
29	1	0	-2.052891	-0.504828	-2.688879
30	6	0	3.088493	-0.816027	0.854160
31	6	0	4.289834	-1.526244	0.820568
32	6	0	4.538323	-2.373787	-0.266375
33	1	0	5.012789	-1.425173	1.623900
34	6	0	2.426842	-1.735467	-1.196285
35	6	0	3.600137	-2.481912	-1.295984
36	1	0	5.464751	-2.938606	-0.308893
37	1	0	3.749822	-3.115557	-2.162858
38	6	0	-3.088493	-0.816027	-0.854160
39	6	0	-4.289834	-1.526245	-0.820568
40	6	0	-2.426842	-1.735467	1.196285
41	6	0	-4.538322	-2.373787	0.266375
42	1	0	-5.012788	-1.425174	-1.623900
43	6	0	-3.600137	-2.481913	1.295984
44	1	0	-5.464750	-2.938607	0.308894
45	1	0	-3.749821	-3.115556	2.162859
46	7	0	-2.191569	-0.932470	0.141025

47	7	0	2.191569	-0.932470	-0.141025
48	6	0	1.329562	-1.740603	-2.255241
49	8	0	0.299143	-0.987845	-1.931154
50	8	0	1.480288	-2.388877	-3.279371
51	6	0	-1.329562	-1.740602	2.255241
52	8	0	-1.480288	-2.388875	3.279372
53	8	0	-0.299142	-0.987846	1.931154
54	1	0	0.670054	3.001977	-3.112712
55	1	0	-0.218765	3.598392	-1.723021
56	1	0	0.218764	3.598392	1.723019
57	1	0	-0.670054	3.001978	3.112711
58	7	0	1.040726	1.983592	-1.257656
59	7	0	-1.040726	1.983592	1.257656
60	1	0	1.680129	1.404992	-1.810503
61	1	0	-1.680129	1.404991	1.810503

E(RTPSSh) = -1524.29036768

Zero-point correction= 0.505581 (Hartree/Particle)

Thermal correction to Energy= 0.534065

Thermal correction to Enthalpy= 0.535010

Thermal correction to Gibbs Free Energy= 0.449138

Sum of electronic and zero-point Energies= -1523.786977

Sum of electronic and thermal Energies= -1523.758492

Sum of electronic and thermal Enthalpies= -1523.757548

Sum of electronic and thermal Free Energies= -1523.843420

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.614377	-1.810066	0.977217
2	6	0	-0.913449	-2.648653	2.002209
3	6	0	0.128926	-1.858537	2.794841
4	6	0	2.298112	-1.981758	1.484647
5	6	0	2.098627	-2.686493	0.135995

6	7	0	1.614377	-1.810066	-0.977217
7	6	0	0.913449	-2.648653	-2.002208
8	6	0	-0.128926	-1.858538	-2.794840
9	6	0	-2.298112	-1.981758	-1.484646
10	6	0	-2.098627	-2.686493	-0.135995
11	6	0	-2.745239	-1.087366	1.641516
12	6	0	2.745239	-1.087366	-1.641516
13	1	0	-0.415726	-3.466930	1.476149
14	1	0	-1.634879	-3.109544	2.692644
15	1	0	3.143826	-1.293489	1.431210
16	1	0	2.553914	-2.750261	2.228485
17	1	0	3.038701	-3.183018	-0.148705
18	1	0	1.353792	-3.476915	0.261907
19	1	0	0.415726	-3.466931	-1.476148
20	1	0	1.634879	-3.109544	-2.692644
21	1	0	-3.143826	-1.293489	-1.431210
22	1	0	-2.553914	-2.750262	-2.228484
23	1	0	-3.038701	-3.183018	0.148706
24	1	0	-1.353792	-3.476915	-0.261906
25	1	0	-3.578121	-1.780454	1.831874
26	1	0	-2.382599	-0.747460	2.619046
27	1	0	3.578121	-1.780454	-1.831874
28	1	0	2.382599	-0.747460	-2.619045
29	6	0	-3.226871	0.128623	0.872521
30	6	0	-4.520681	0.643109	0.972970
31	6	0	-4.832307	1.811381	0.266130
32	1	0	-5.266385	0.149502	1.588536
33	6	0	-2.602343	1.829138	-0.610231
34	6	0	-3.866419	2.413931	-0.542561
35	1	0	-5.829523	2.235152	0.337226
36	1	0	-4.062158	3.305398	-1.127702
37	6	0	3.226871	0.128623	-0.872521
38	6	0	4.520681	0.643108	-0.972970
39	6	0	2.602343	1.829138	0.610231
40	6	0	4.832307	1.811381	-0.266130
41	1	0	5.266385	0.149502	-1.588536

42	6	0	3.866419	2.413931	0.542561
43	1	0	5.829523	2.235152	-0.337225
44	1	0	4.062158	3.305398	1.127702
45	7	0	2.301499	0.725272	-0.103585
46	7	0	-2.301499	0.725272	0.103585
47	6	0	-1.499243	2.337354	-1.538878
48	8	0	-0.423666	1.582043	-1.521867
49	8	0	-1.710158	3.325882	-2.223736
50	6	0	1.499242	2.337354	1.538878
51	8	0	1.710159	3.325882	2.223737
52	8	0	0.423666	1.582044	1.521866
53	1	0	-0.614070	-2.536338	-3.512216
54	1	0	0.351850	-1.064987	-3.376541
55	1	0	-0.351850	-1.064987	3.376541
56	1	0	0.614070	-2.536337	3.512217
57	7	0	-1.114796	-1.197136	-1.909286
58	7	0	1.114796	-1.197135	1.909286
59	70	0	0.000000	0.039511	0.000000
60	1	0	1.438756	-0.357797	2.390010
61	1	0	-1.438756	-0.357797	-2.390009

E(RTPSSh) = -1524.27382914

Zero-point correction= 0.505992 (Hartree/Particle)

Thermal correction to Energy= 0.534209

Thermal correction to Enthalpy= 0.535153

Thermal correction to Gibbs Free Energy= 0.449860

Sum of electronic and zero-point Energies= -1523.773565

Sum of electronic and thermal Energies= -1523.745347

Sum of electronic and thermal Enthalpies= -1523.744403

Sum of electronic and thermal Free Energies= -1523.829696

[Lu(dodpa)]

F1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	71	0	0.000000	0.086985	0.000000
2	7	0	1.883819	1.529200	1.085786
3	6	0	1.325372	2.501138	2.069312
4	6	0	0.030675	2.005008	2.713233
5	6	0	-1.713664	2.793830	1.076514
6	6	0	-2.637103	2.257948	-0.020533
7	7	0	-1.883819	1.529200	-1.085786
8	6	0	-1.325372	2.501138	-2.069312
9	6	0	-0.030675	2.005008	-2.713233
10	6	0	1.713664	2.793830	-1.076514
11	6	0	2.637103	2.257948	0.020533
12	6	0	2.778990	0.537613	1.756859
13	6	0	-2.778990	0.537613	-1.756859
14	1	0	1.132055	3.436178	1.533749
15	1	0	2.063118	2.733750	2.850499
16	1	0	0.211565	1.086464	3.278525
17	1	0	-0.338461	2.767261	3.414272
18	1	0	-0.984260	3.498505	0.662136
19	1	0	-2.310279	3.346868	1.816499
20	1	0	-3.344920	1.554864	0.429160
21	1	0	-3.225915	3.078516	-0.454843
22	1	0	-1.132055	3.436178	-1.533749
23	1	0	-2.063118	2.733750	-2.850499
24	1	0	-0.211565	1.086464	-3.278525
25	1	0	0.338461	2.767261	-3.414272
26	1	0	0.984260	3.498505	-0.662136
27	1	0	2.310279	3.346868	-1.816499
28	1	0	3.344920	1.554864	-0.429160
29	1	0	3.225915	3.078516	0.454843
30	1	0	3.687388	1.024769	2.141160
31	1	0	2.232289	0.120685	2.610769
32	1	0	-3.687388	1.024769	-2.141160
33	1	0	-2.232289	0.120685	-2.610769
34	6	0	3.131397	-0.591621	0.803561

35	6	0	4.312963	-1.332635	0.848592
36	6	0	4.491267	-2.364923	-0.082027
37	1	0	5.075076	-1.114414	1.590123
38	6	0	2.355359	-1.836032	-1.025112
39	6	0	3.508273	-2.620202	-1.041064
40	1	0	5.401098	-2.957203	-0.060669
41	1	0	3.607790	-3.396611	-1.791223
42	6	0	-3.131397	-0.591621	-0.803561
43	6	0	-4.312963	-1.332635	-0.848592
44	6	0	-2.355359	-1.836032	1.025112
45	6	0	-4.491267	-2.364923	0.082027
46	1	0	-5.075076	-1.114414	-1.590123
47	6	0	-3.508273	-2.620202	1.041064
48	1	0	-5.401098	-2.957203	0.060669
49	1	0	-3.607790	-3.396611	1.791223
50	7	0	-2.188773	-0.856470	0.116694
51	7	0	2.188773	-0.856470	-0.116694
52	6	0	1.211888	-1.990786	-2.026011
53	8	0	0.194667	-1.193610	-1.775543
54	8	0	1.325503	-2.784316	-2.947285
55	6	0	-1.211888	-1.990786	2.026011
56	8	0	-1.325503	-2.784317	2.947285
57	8	0	-0.194667	-1.193610	1.775543
58	7	0	-0.980683	1.664441	1.682555
59	7	0	0.980683	1.664441	-1.682555
60	1	0	-1.660799	1.039585	2.120897
61	1	0	1.660799	1.039585	-2.120896

E(RTPSSh) = -1524.84410335

Zero-point correction= 0.504749 (Hartree/Particle)

Thermal correction to Energy= 0.533211

Thermal correction to Enthalpy= 0.534155

Thermal correction to Gibbs Free Energy= 0.448241

Sum of electronic and zero-point Energies= -1524.342961

Sum of electronic and thermal Energies= -1524.314499

Sum of electronic and thermal Enthalpies= -1524.313554

Sum of electronic and thermal Free Energies= -1524.399468

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.000000	0.032300
2	7	0	0.000000	2.183989	1.398572
3	6	0	1.017883	2.133707	2.491612
4	6	0	2.286291	1.349865	2.138369
5	6	0	1.883852	-1.073454	2.641108
6	6	0	1.360961	-2.359344	1.992663
7	7	0	0.000000	-2.183989	1.398572
8	6	0	-1.017883	-2.133707	2.491612
9	6	0	-2.286291	-1.349865	2.138369
10	6	0	-1.883852	1.073454	2.641108
11	6	0	-1.360961	2.359344	1.992663
12	6	0	0.273953	3.295388	0.434874
13	6	0	-0.273953	-3.295388	0.434874
14	1	0	0.545784	1.655501	3.354414
15	1	0	1.289706	3.152688	2.804448
16	1	0	2.856667	1.866719	1.365140
17	1	0	2.924043	1.295811	3.031782
18	1	0	1.232546	-0.735038	3.454072
19	1	0	2.868479	-1.275815	3.086451
20	1	0	2.035582	-2.636621	1.176444
21	1	0	1.369566	-3.177456	2.727966
22	1	0	-0.545784	-1.655501	3.354414
23	1	0	-1.289706	-3.152688	2.804448
24	1	0	-2.856667	-1.866719	1.365140
25	1	0	-2.924043	-1.295811	3.031782
26	1	0	-1.232546	0.735038	3.454072
27	1	0	-2.868479	1.275815	3.086451
28	1	0	-2.035582	2.636621	1.176444
29	1	0	-1.369566	3.177456	2.727966

30	1	0	-0.645021	3.450682	-0.141732
31	1	0	0.500441	4.229779	0.968728
32	1	0	0.645021	-3.450682	-0.141732
33	1	0	-0.500441	-4.229779	0.968728
34	6	0	1.376294	2.954064	-0.550898
35	6	0	2.205794	3.897133	-1.161081
36	6	0	3.136795	3.456588	-2.110679
37	1	0	2.126197	4.949540	-0.907052
38	6	0	2.384730	1.212245	-1.751031
39	6	0	3.237483	2.096098	-2.411420
40	1	0	3.785991	4.175002	-2.602134
41	1	0	3.952465	1.704014	-3.125922
42	6	0	-1.376294	-2.954064	-0.550898
43	6	0	-2.205794	-3.897133	-1.161081
44	6	0	-2.384730	-1.212245	-1.751031
45	6	0	-3.136795	-3.456588	-2.110679
46	1	0	-2.126197	-4.949540	-0.907052
47	6	0	-3.237483	-2.096098	-2.411420
48	1	0	-3.785991	-4.175002	-2.602134
49	1	0	-3.952465	-1.704014	-3.125922
50	7	0	-1.476543	-1.650124	-0.857952
51	7	0	1.476543	1.650124	-0.857952
52	6	0	2.436763	-0.302952	-1.937013
53	8	0	1.559260	-0.946469	-1.195498
54	8	0	3.266206	-0.785589	-2.692222
55	6	0	-2.436763	0.302952	-1.937013
56	8	0	-3.266206	0.785589	-2.692222
57	8	0	-1.559260	0.946469	-1.195498
58	7	0	-1.950078	0.000386	1.626121
59	7	0	1.950078	-0.000386	1.626121
60	1	0	2.653509	-0.273387	0.936282
61	1	0	-2.653509	0.273387	0.936282

E(RTPSSh) = -1524.84338443

Zero-point correction= 0.505155 (Hartree/Particle)

Thermal correction to Energy= 0.533701

Thermal correction to Enthalpy= 0.534645

Thermal correction to Gibbs Free Energy= 0.448851

Sum of electronic and zero-point Energies= -1524.342108

Sum of electronic and thermal Energies= -1524.313562

Sum of electronic and thermal Enthalpies= -1524.312618

Sum of electronic and thermal Free Energies= -1524.398412

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.000000	0.078758
2	7	0	0.121398	2.291762	1.179484
3	6	0	1.475346	2.404815	1.792279
4	6	0	1.844442	1.217654	2.685701
5	6	0	1.442852	-1.224771	2.897255
6	6	0	1.004711	-2.485569	2.140868
7	7	0	-0.121398	-2.291762	1.179484
8	6	0	-1.475346	-2.404815	1.792279
9	6	0	-1.844442	-1.217654	2.685701
10	6	0	-1.442852	1.224771	2.897255
11	6	0	-1.004711	2.485569	2.140868
12	6	0	0.000000	3.306761	0.086419
13	6	0	0.000000	-3.306761	0.086419
14	1	0	1.568228	3.334722	2.374730
15	1	0	2.181650	2.450055	0.959076
16	1	0	0.697785	-0.927310	3.637931
17	1	0	2.361778	-1.460887	3.453146
18	1	0	1.857826	-2.843790	1.556146
19	1	0	0.760128	-3.274602	2.867824
20	1	0	-1.568228	-3.334722	2.374730
21	1	0	-2.181650	-2.450055	0.959076
22	1	0	-0.697785	0.927310	3.637931
23	1	0	-2.361778	1.460887	3.453146
24	1	0	-1.857826	2.843790	1.556146

25	1	0	-0.760128	3.274602	2.867824
26	1	0	-0.094705	4.323007	0.495085
27	1	0	0.920913	3.253269	-0.503686
28	1	0	0.094705	-4.323007	0.495085
29	1	0	-0.920913	-3.253269	-0.503686
30	6	0	-1.164640	2.970778	-0.822491
31	6	0	-1.910141	3.906117	-1.542370
32	6	0	-2.922631	3.446146	-2.393513
33	1	0	-1.703906	4.967424	-1.445859
34	6	0	-2.398139	1.203947	-1.739931
35	6	0	-3.179413	2.076590	-2.495949
36	1	0	-3.510696	4.157367	-2.965738
37	1	0	-3.957624	1.670816	-3.132433
38	6	0	1.164640	-2.970778	-0.822491
39	6	0	1.910141	-3.906117	-1.542370
40	6	0	2.398139	-1.203947	-1.739931
41	6	0	2.922631	-3.446146	-2.393513
42	1	0	1.703906	-4.967424	-1.445859
43	6	0	3.179413	-2.076590	-2.495949
44	1	0	3.510696	-4.157367	-2.965738
45	1	0	3.957624	-1.670816	-3.132433
46	7	0	1.418944	-1.654942	-0.932718
47	7	0	-1.418944	1.654942	-0.932718
48	6	0	-2.581089	-0.309302	-1.737599
49	8	0	-1.705577	-0.930028	-0.974848
50	8	0	-3.483822	-0.812105	-2.388731
51	6	0	2.581089	0.309302	-1.737599
52	8	0	3.483822	0.812105	-2.388731
53	8	0	1.705577	0.930028	-0.974848
54	1	0	-2.889277	-1.330767	3.002620
55	1	0	-1.243861	-1.206264	3.598065
56	1	0	1.243861	1.206264	3.598065
57	1	0	2.889277	1.330767	3.002620
58	7	0	-1.628040	0.076677	1.980747
59	7	0	1.628040	-0.076677	1.980747
60	1	0	-2.452578	0.253462	1.399202

61	1	0	2.452578	-0.253462	1.399202

E(RTPSSh) = -1524.84502688

Zero-point correction= 0.506093 (Hartree/Particle)

Thermal correction to Energy= 0.534448

Thermal correction to Enthalpy= 0.535392

Thermal correction to Gibbs Free Energy= 0.450542

Sum of electronic and zero-point Energies= -1524.341259

Sum of electronic and thermal Energies= -1524.312904

Sum of electronic and thermal Enthalpies= -1524.311960

Sum of electronic and thermal Free Energies= -1524.396810

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.000000	0.027690
2	7	0	-0.525245	1.811233	-1.808278
3	6	0	-1.701447	1.406075	-2.643413
4	6	0	-2.732524	0.602232	-1.850253
5	6	0	-2.027423	-1.831204	-1.984921
6	6	0	-0.672827	-1.987724	-2.688485
7	7	0	0.525245	-1.811233	-1.808278
8	6	0	1.701447	-1.406075	-2.643413
9	6	0	2.732524	-0.602232	-1.850253
10	6	0	2.027423	1.831204	-1.984921
11	6	0	0.672827	1.987724	-2.688485
12	6	0	-0.866583	3.075427	-1.081616
13	6	0	0.866583	-3.075427	-1.081616
14	1	0	-1.327738	0.792524	-3.466869
15	1	0	-2.182461	2.284734	-3.097276
16	1	0	-2.197344	-2.664145	-1.299921
17	1	0	-2.812064	-1.880372	-2.753703
18	1	0	-0.640776	-2.968057	-3.187712
19	1	0	-0.599209	-1.233092	-3.476299

20	1	0	1.327738	-0.792524	-3.466869
21	1	0	2.182461	-2.284734	-3.097276
22	1	0	2.197344	2.664145	-1.299921
23	1	0	2.812064	1.880372	-2.753703
24	1	0	0.640776	2.968057	-3.187712
25	1	0	0.599209	1.233092	-3.476299
26	1	0	-0.827338	3.931529	-1.771368
27	1	0	-1.905893	2.984267	-0.743888
28	1	0	0.827338	-3.931529	-1.771368
29	1	0	1.905893	-2.984267	-0.743888
30	6	0	0.000000	3.329962	0.137328
31	6	0	0.237807	4.600413	0.664839
32	6	0	0.998699	4.706291	1.835849
33	1	0	-0.162264	5.485186	0.179277
34	6	0	1.265055	2.325286	1.831542
35	6	0	1.526986	3.557619	2.428922
36	1	0	1.187940	5.683563	2.269673
37	1	0	2.140087	3.586044	3.322622
38	6	0	0.000000	-3.329962	0.137328
39	6	0	-0.237807	-4.600413	0.664839
40	6	0	-1.265055	-2.325286	1.831542
41	6	0	-0.998699	-4.706291	1.835849
42	1	0	0.162264	-5.485186	0.179277
43	6	0	-1.526986	-3.557619	2.428922
44	1	0	-1.187940	-5.683563	2.269673
45	1	0	-2.140087	-3.586044	3.322622
46	7	0	-0.501190	-2.231204	0.724228
47	7	0	0.501190	2.231204	0.724228
48	6	0	1.869809	1.012472	2.328893
49	8	0	1.569976	-0.014044	1.564307
50	8	0	2.585019	1.025981	3.318276
51	6	0	-1.869809	-1.012472	2.328893
52	8	0	-2.585019	-1.025981	3.318276
53	8	0	-1.569976	0.014044	1.564307
54	1	0	3.554968	-0.320425	-2.523605
55	1	0	3.164993	-1.214439	-1.051895

56	1	0	-3.164993	1.214439	-1.051895
57	1	0	-3.554968	0.320425	-2.523605
58	7	0	2.126679	0.580506	-1.196139
59	7	0	-2.126679	-0.580506	-1.196139
60	1	0	-2.668969	-0.770770	-0.353463
61	1	0	2.668969	0.770770	-0.353463

E(RTPSSh) = -1524.82807957

Zero-point correction= 0.505840 (Hartree/Particle)

Thermal correction to Energy= 0.534007

Thermal correction to Enthalpy= 0.534951

Thermal correction to Gibbs Free Energy= 0.450692

Sum of electronic and zero-point Energies= -1524.327430

Sum of electronic and thermal Energies= -1524.299263

Sum of electronic and thermal Enthalpies= -1524.298319

Sum of electronic and thermal Free Energies= -1524.382579

Complejos de H_2Me_2DODPA

Las geometrías optimizadas en disolución se corresponden con las siguientes conformaciones:

- F1: Λ(λλλλ)
- F2: Δ(λλλλ)
- F3: Λ(δλδλ)
- F4: Λ(λδλδ)

[$La(Me_2dodpa)$]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-0.002338	0.186332	-0.004208
2	7	0	1.930395	-1.660756	-1.009686
3	6	0	1.300775	-2.703244	-1.870025
4	6	0	0.131183	-2.187181	-2.705612
5	6	0	-1.728585	-2.796409	-1.233826
6	6	0	-2.648244	-2.327683	-0.108838
7	7	0	-1.926406	-1.658991	1.015907
8	6	0	-1.291505	-2.688348	1.888431
9	6	0	-0.125867	-2.157283	2.720414
10	6	0	1.737243	-2.770584	1.255141
11	6	0	2.654445	-2.312507	0.123674
12	6	0	2.917173	-0.899276	-1.821482
13	6	0	-2.917134	-0.894846	1.820361
14	1	0	0.970397	-3.517006	-1.221076
15	1	0	2.050202	-3.136850	-2.548292
16	1	0	0.461310	-1.360672	-3.343497
17	1	0	-0.201431	-2.995572	-3.375781
18	1	0	-0.991276	-3.500319	-0.842310
19	1	0	-2.333150	-3.351027	-1.968551
20	1	0	-3.379059	-1.616599	-0.500415
21	1	0	-3.214492	-3.191164	0.270637
22	1	0	-0.955615	-3.506942	1.248580
23	1	0	-2.039378	-3.119079	2.570202

24	1	0	-0.461236	-1.327025	3.350561
25	1	0	0.210259	-2.958003	3.398011
26	1	0	1.002882	-3.482282	0.871960
27	1	0	2.344903	-3.315045	1.994926
28	1	0	3.383582	-1.594937	0.506260
29	1	0	3.222958	-3.179343	-0.244714
30	1	0	3.743579	-1.551497	-2.140515
31	1	0	2.413487	-0.550876	-2.730376
32	1	0	-3.742456	-1.547444	2.141435
33	1	0	-2.416613	-0.539877	2.728459
34	6	0	3.460414	0.296415	-1.068837
35	6	0	4.753397	0.786417	-1.280710
36	6	0	5.172721	1.911084	-0.567124
37	1	0	5.413853	0.293118	-1.986126
38	6	0	3.027491	1.956427	0.505321
39	6	0	4.298914	2.506332	0.344487
40	1	0	6.171489	2.309781	-0.715003
41	1	0	4.575255	3.374402	0.931350
42	6	0	-3.461890	0.296479	1.061989
43	6	0	-4.753336	0.789082	1.277442
44	6	0	-3.030930	1.954124	-0.515253
45	6	0	-5.172617	1.914172	0.564637
46	1	0	-5.412067	0.298229	1.986172
47	6	0	-4.300353	2.507187	-0.349912
48	1	0	-6.169728	2.315636	0.716171
49	1	0	-4.576089	3.376527	-0.935168
50	7	0	-2.625662	0.872101	0.179649
51	7	0	2.622196	0.875214	-0.190485
52	6	0	2.020506	2.545605	1.482690
53	8	0	0.875227	1.941702	1.513530
54	8	0	2.355666	3.526660	2.159555
55	6	0	-2.025492	2.543195	-1.494429
56	8	0	-2.361400	3.525485	-2.169194
57	8	0	-0.880532	1.938937	-1.528209
58	7	0	-1.012673	-1.678320	-1.899158
59	7	0	1.016419	-1.649546	1.910784

60	6	0	1.938358	-0.932767	2.825261
61	1	0	2.796281	-0.553705	2.267447
62	1	0	1.415764	-0.083637	3.269538
63	1	0	2.298154	-1.599877	3.623184
64	6	0	-1.937060	-0.971464	-2.819060
65	1	0	-2.798819	-0.595026	-2.265504
66	1	0	-1.418117	-0.120919	-3.265230
67	1	0	-2.290768	-1.643627	-3.615438

E(RTPSSh) = -1595.08174720

Zero-point correction= 0.559123 (Hartree/Particle)

Thermal correction to Energy= 0.590922

Thermal correction to Enthalpy= 0.591866

Thermal correction to Gibbs Free Energy= 0.498892

Sum of electronic and zero-point Energies= -1594.522622

Sum of electronic and thermal Energies= -1594.490824

Sum of electronic and thermal Enthalpies= -1594.489880

Sum of electronic and thermal Free Energies= -1594.582854

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-0.007284	0.279924	-0.023367
2	7	0	1.583999	-1.495621	1.516143
3	6	0	2.175707	-2.584037	0.672306
4	6	0	2.600712	-2.168884	-0.740887
5	6	0	0.570260	-2.672950	-2.005408
6	6	0	-0.761643	-2.151163	-2.530958
7	7	0	-1.608135	-1.503115	-1.479018
8	6	0	-2.212138	-2.567087	-0.616447
9	6	0	-2.626775	-2.126386	0.787158
10	6	0	-0.605894	-2.632843	2.055809
11	6	0	0.734652	-2.118311	2.578429
12	6	0	2.657513	-0.711507	2.190505

13	6	0	-2.673410	-0.716315	-2.163670
14	1	0	1.439547	-3.387689	0.606698
15	1	0	3.051219	-3.011033	1.183490
16	1	0	3.392664	-1.419876	-0.693312
17	1	0	3.028044	-3.055450	-1.237138
18	1	0	0.399305	-3.346481	-1.162506
19	1	0	1.042365	-3.275083	-2.797648
20	1	0	-0.586036	-1.408104	-3.312767
21	1	0	-1.308428	-2.984434	-2.996376
22	1	0	-1.485899	-3.378737	-0.540731
23	1	0	-3.094086	-2.990694	-1.118734
24	1	0	-3.414621	-1.373378	0.732444
25	1	0	-3.058605	-3.002624	1.297542
26	1	0	-0.442386	-3.321945	1.224176
27	1	0	-1.089931	-3.214881	2.855822
28	1	0	0.569647	-1.365179	3.352519
29	1	0	1.270914	-2.953533	3.053174
30	1	0	2.178870	-0.119683	2.979718
31	1	0	3.378502	-1.380932	2.681016
32	1	0	-2.188335	-0.131256	-2.953858
33	1	0	-3.396831	-1.385209	-2.650108
34	6	0	3.379067	0.251052	1.275476
35	6	0	4.732084	0.565807	1.441989
36	6	0	5.302882	1.540166	0.619804
37	1	0	5.320990	0.059891	2.199821
38	6	0	3.178511	1.781964	-0.466222
39	6	0	4.515000	2.164702	-0.348412
40	1	0	6.349996	1.803362	0.732403
41	1	0	4.906491	2.926512	-1.012292
42	6	0	-3.386622	0.256155	-1.248877
43	6	0	-4.753135	0.531959	-1.360395
44	6	0	-3.146909	1.837865	0.445293
45	6	0	-5.313120	1.505164	-0.528455
46	1	0	-5.362273	-0.005259	-2.079581
47	6	0	-4.499792	2.175337	0.386441
48	1	0	-6.372321	1.733575	-0.594123

49	1	0	-4.883515	2.939350	1.052294
50	7	0	-2.612046	0.895700	-0.352444
51	7	0	2.629577	0.846472	0.333006
52	6	0	2.259331	2.390859	-1.515668
53	8	0	1.069787	1.879918	-1.553801
54	8	0	2.699613	3.292104	-2.240846
55	6	0	-2.190311	2.508270	1.419589
56	8	0	-2.626367	3.397689	2.161063
57	8	0	-0.976621	2.058292	1.381935
58	7	0	-1.516566	-1.552600	1.592542
59	7	0	1.499188	-1.597670	-1.563877
60	6	0	-2.102030	-0.874457	2.774457
61	1	0	-1.318422	-0.389854	3.359263
62	1	0	-2.806337	-0.109832	2.442759
63	1	0	-2.634892	-1.592820	3.416109
64	6	0	2.099793	-0.956221	-2.758593
65	1	0	1.326782	-0.479323	-3.363297
66	1	0	2.806285	-0.188873	-2.439893
67	1	0	2.630670	-1.697203	-3.375833

E(RTPSSh) = -1595.07807893

Zero-point correction= 0.559147 (Hartree/Particle)

Thermal correction to Energy= 0.590868

Thermal correction to Enthalpy= 0.591812

Thermal correction to Gibbs Free Energy= 0.499107

Sum of electronic and zero-point Energies= -1594.519436

Sum of electronic and thermal Energies= -1594.487715

Sum of electronic and thermal Enthalpies= -1594.486771

Sum of electronic and thermal Free Energies= -1594.579476

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	57	0	0.000000	0.171126	0.000000

2	7	0	1.751473	-1.235348	-1.575907
3	6	0	0.958933	-1.880305	-2.662962
4	6	0	-0.204230	-2.759239	-2.192334
5	6	0	-1.861646	-2.919588	-0.384642
6	6	0	-2.570543	-2.191655	0.769956
7	7	0	-1.751474	-1.235348	1.575907
8	6	0	-0.958933	-1.880305	2.662961
9	6	0	0.204229	-2.759240	2.192334
10	6	0	1.861644	-2.919588	0.384642
11	6	0	2.570542	-2.191656	-0.769957
12	6	0	2.672732	-0.235626	-2.207577
13	6	0	-2.672732	-0.235626	2.207577
14	1	0	1.614452	-2.489946	-3.305999
15	1	0	0.562958	-1.067792	-3.281629
16	1	0	-1.107213	-3.606066	0.000206
17	1	0	-2.622888	-3.542386	-0.883842
18	1	0	-3.402733	-1.614787	0.356923
19	1	0	-3.012236	-2.954901	1.430364
20	1	0	-1.614453	-2.489946	3.305999
21	1	0	-0.562959	-1.067793	3.281630
22	1	0	1.107211	-3.606066	-0.000208
23	1	0	2.622886	-3.542388	0.883841
24	1	0	3.402732	-1.614789	-0.356923
25	1	0	3.012235	-2.954901	-1.430364
26	1	0	3.464183	-0.740488	-2.781443
27	1	0	2.077536	0.350931	-2.918129
28	1	0	-3.464183	-0.740487	2.781444
29	1	0	-2.077536	0.350931	2.918129
30	6	0	3.276187	0.712154	-1.186347
31	6	0	4.550646	1.269857	-1.304215
32	6	0	4.974606	2.182690	-0.329969
33	1	0	5.195538	1.004212	-2.136108
34	6	0	2.880281	1.887531	0.798887
35	6	0	4.135456	2.495819	0.741026
36	1	0	5.959097	2.634672	-0.405191
37	1	0	4.421171	3.182319	1.530039

38	6	0	-3.276186	0.712155	1.186347
39	6	0	-4.550645	1.269858	1.304215
40	6	0	-2.880280	1.887531	-0.798887
41	6	0	-4.974606	2.182691	0.329969
42	1	0	-5.195538	1.004213	2.136108
43	6	0	-4.135455	2.495820	-0.741026
44	1	0	-5.959096	2.634674	0.405191
45	1	0	-4.421170	3.182320	-1.530039
46	7	0	-2.472370	1.028998	0.155306
47	7	0	2.472371	1.028998	-0.155306
48	6	0	1.909772	2.118211	1.959643
49	8	0	0.769746	1.480882	1.828938
50	8	0	2.264698	2.827250	2.890091
51	6	0	-1.909771	2.118211	-1.959643
52	8	0	-2.264697	2.827250	-2.890091
53	8	0	-0.769746	1.480881	-1.828938
54	1	0	0.689608	-3.172632	3.089430
55	1	0	-0.166966	-3.616341	1.628618
56	1	0	0.166965	-3.616341	-1.628619
57	1	0	-0.689609	-3.172631	-3.089431
58	7	0	1.196722	-2.020631	1.360441
59	7	0	-1.196723	-2.020630	-1.360441
60	6	0	2.210146	-1.409107	2.259075
61	1	0	2.922987	-0.824173	1.676016
62	1	0	1.722482	-0.732378	2.962598
63	1	0	2.754070	-2.187983	2.815287
64	6	0	-2.210146	-1.409106	-2.259075
65	1	0	-2.922987	-0.824171	-1.676015
66	1	0	-1.722482	-0.732377	-2.962597
67	1	0	-2.754071	-2.187981	-2.815287

E(RTPSSh) = -1595.06254097

Zero-point correction= 0.559816 (Hartree/Particle)

Thermal correction to Energy= 0.591477

Thermal correction to Enthalpy= 0.592421

Thermal correction to Gibbs Free Energy= 0.499781

Sum of electronic and zero-point Energies= -1594.512410

Sum of electronic and thermal Energies= -1594.480749

Sum of electronic and thermal Enthalpies= -1594.479804

Sum of electronic and thermal Free Energies= -1594.572445

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.329961	1.812546	-1.852350
2	6	0	-1.347925	1.313096	-2.823224
3	6	0	-2.606036	0.718175	-2.187189
4	6	0	-2.253049	-1.715228	-1.784084
5	6	0	-0.972074	-2.020734	-2.571682
6	7	0	0.329961	-1.812546	-1.852350
7	6	0	1.347925	-1.313096	-2.823224
8	6	0	2.606036	-0.718175	-2.187189
9	6	0	2.253049	1.715228	-1.784084
10	6	0	0.972074	2.020734	-2.571682
11	6	0	-0.815517	3.099244	-1.265945
12	6	0	0.815517	-3.099244	-1.265945
13	1	0	-0.858069	0.562229	-3.442798
14	1	0	-1.662579	2.121050	-3.503901
15	1	0	-2.350215	-2.424979	-0.961006
16	1	0	-3.096762	-1.902085	-2.471111
17	1	0	-1.045689	-3.065973	-2.905780
18	1	0	-0.951320	-1.419627	-3.483507
19	1	0	0.858069	-0.562229	-3.442798
20	1	0	1.662579	-2.121050	-3.503901
21	1	0	2.350215	2.424979	-0.961006
22	1	0	3.096762	1.902085	-2.471111
23	1	0	1.045689	3.065973	-2.905780
24	1	0	0.951320	1.419627	-3.483507
25	1	0	-0.843450	3.881803	-2.039944
26	1	0	-1.849489	2.943559	-0.935670

27	1	0	0.843450	-3.881803	-2.039944
28	1	0	1.849489	-2.943559	-0.935670
29	6	0	0.000000	3.564377	-0.076849
30	6	0	0.245387	4.909917	0.199404
31	6	0	0.965755	5.235797	1.355977
32	1	0	-0.117640	5.685676	-0.467870
33	6	0	1.188701	2.892221	1.816572
34	6	0	1.451662	4.216358	2.174387
35	1	0	1.159914	6.276355	1.598268
36	1	0	2.041145	4.405152	3.064647
37	6	0	0.000000	-3.564377	-0.076849
38	6	0	-0.245387	-4.909917	0.199404
39	6	0	-1.188701	-2.892221	1.816572
40	6	0	-0.965755	-5.235797	1.355977
41	1	0	0.117640	-5.685676	-0.467870
42	6	0	-1.451662	-4.216358	2.174387
43	1	0	-1.159914	-6.276355	1.598268
44	1	0	-2.041145	-4.405152	3.064647
45	7	0	-0.451759	-2.586435	0.729527
46	7	0	0.451759	2.586435	0.729527
47	6	0	1.795670	1.713941	2.580092
48	8	0	1.530274	0.555110	2.035998
49	8	0	2.490617	1.947262	3.558857
50	6	0	-1.795670	-1.713941	2.580092
51	8	0	-2.490617	-1.947262	3.558857
52	8	0	-1.530274	-0.555110	2.035998
53	1	0	3.257588	-0.360791	-3.001612
54	1	0	3.165390	-1.509964	-1.679920
55	1	0	-3.165390	1.509964	-1.679920
56	1	0	-3.257588	0.360791	-3.001612
57	7	0	2.383335	0.357271	-1.184472
58	7	0	-2.383335	-0.357271	-1.184472
59	6	0	3.588104	0.390425	-0.304212
60	1	0	3.488978	1.189620	0.428662
61	1	0	3.670684	-0.552466	0.240770
62	1	0	4.501789	0.549049	-0.896674

63	6	0	-3.588104	-0.390425	-0.304212
64	1	0	-3.488978	-1.189620	0.428662
65	1	0	-3.670684	0.552466	0.240770
66	1	0	-4.501789	-0.549049	-0.896674
67	57	0	0.000000	0.000000	0.321761

E(RTPSSh) = -1595.05844321

Zero-point correction= 0.560022 (Hartree/Particle)

Thermal correction to Energy= 0.591789

Thermal correction to Enthalpy= 0.592733

Thermal correction to Gibbs Free Energy= 0.499956

Sum of electronic and zero-point Energies= -1594.506137

Sum of electronic and thermal Energies= -1594.474370

Sum of electronic and thermal Enthalpies= -1594.473425

Sum of electronic and thermal Free Energies= -1594.566203

[Nd(Me_2dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	0.000000	0.075559	0.000000
2	7	0	-1.888487	-1.620896	1.069383
3	6	0	-1.281033	-2.663557	1.942973
4	6	0	-0.070600	-2.173362	2.738651
5	6	0	1.739978	-2.764568	1.185322
6	6	0	2.639375	-2.270831	0.047181
7	7	0	1.888487	-1.620896	-1.069383
8	6	0	1.281033	-2.663557	-1.942973
9	6	0	0.070601	-2.173362	-2.738651
10	6	0	-1.739978	-2.764568	-1.185322
11	6	0	-2.639375	-2.270832	-0.047181
12	6	0	-2.823791	-0.770403	1.865588

13	6	0	2.823791	-0.770403	-1.865588
14	1	0	-0.995266	-3.504701	1.305441
15	1	0	-2.029368	-3.055748	2.648765
16	1	0	-0.365398	-1.350244	3.397961
17	1	0	0.270713	-2.993386	3.392000
18	1	0	0.986717	-3.451956	0.787618
19	1	0	2.357945	-3.348948	1.886815
20	1	0	3.355510	-1.541084	0.431077
21	1	0	3.223161	-3.121487	-0.337281
22	1	0	0.995266	-3.504702	-1.305441
23	1	0	2.029368	-3.055748	-2.648765
24	1	0	0.365398	-1.350245	-3.397961
25	1	0	-0.270713	-2.993387	-3.392000
26	1	0	-0.986716	-3.451956	-0.787618
27	1	0	-2.357944	-3.348949	-1.886815
28	1	0	-3.355510	-1.541084	-0.431077
29	1	0	-3.223161	-3.121487	0.337281
30	1	0	-3.686636	-1.362048	2.208377
31	1	0	-2.288269	-0.433820	2.761635
32	1	0	3.686636	-1.362048	-2.208377
33	1	0	2.288269	-0.433820	-2.761635
34	6	0	-3.291793	0.443044	1.080622
35	6	0	-4.524943	1.064450	1.283145
36	6	0	-4.834504	2.198911	0.522373
37	1	0	-5.226643	0.676916	2.015389
38	6	0	-2.720194	1.981966	-0.585771
39	6	0	-3.928107	2.663560	-0.432219
40	1	0	-5.784675	2.703935	0.667955
41	1	0	-4.126841	3.523494	-1.061837
42	6	0	3.291793	0.443044	-1.080622
43	6	0	4.524943	1.064450	-1.283145
44	6	0	2.720194	1.981966	0.585771
45	6	0	4.834504	2.198910	-0.522373
46	1	0	5.226644	0.676916	-2.015389
47	6	0	3.928107	2.663561	0.432219
48	1	0	5.784675	2.703935	-0.667955

49	1	0	4.126841	3.523494	1.061837
50	7	0	2.419160	0.907809	-0.169647
51	7	0	-2.419160	0.907809	0.169646
52	6	0	-1.683018	2.371380	-1.639520
53	8	0	-0.597815	1.633881	-1.601971
54	8	0	-1.943725	3.277408	-2.416929
55	6	0	1.683018	2.371381	1.639520
56	8	0	1.943725	3.277408	2.416929
57	8	0	0.597815	1.633881	1.601971
58	7	0	1.046432	-1.664672	1.899865
59	7	0	-1.046432	-1.664672	-1.899865
60	6	0	-2.003999	-0.965486	-2.795775
61	1	0	-2.827877	-0.551984	-2.212067
62	1	0	-1.495318	-0.136138	-3.288918
63	1	0	-2.409983	-1.656198	-3.550838
64	6	0	2.003999	-0.965486	2.795775
65	1	0	2.827878	-0.551983	2.212067
66	1	0	1.495318	-0.136137	3.288917
67	1	0	2.409983	-1.656198	3.550838

E(RTPSSh) = -1596.98143287

Zero-point correction= 0.559318 (Hartree/Particle)

Thermal correction to Energy= 0.590983

Thermal correction to Enthalpy= 0.591927

Thermal correction to Gibbs Free Energy= 0.499777

Sum of electronic and zero-point Energies= -1596.428350

Sum of electronic and thermal Energies= -1596.396684

Sum of electronic and thermal Enthalpies= -1596.395740

Sum of electronic and thermal Free Energies= -1596.487890

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	60	0	0.000000	0.164134	0.000000

2	7	0	-1.571855	-1.489062	-1.517057
3	6	0	-2.192834	-2.557732	-0.675739
4	6	0	-2.614679	-2.138895	0.734051
5	6	0	-0.603355	-2.670133	2.033386
6	6	0	0.729595	-2.136762	2.570336
7	7	0	1.571855	-1.489062	1.517056
8	6	0	2.192834	-2.557732	0.675739
9	6	0	2.614679	-2.138895	-0.734051
10	6	0	0.603355	-2.670132	-2.033385
11	6	0	-0.729595	-2.136763	-2.570337
12	6	0	-2.617871	-0.644550	-2.175581
13	6	0	2.617871	-0.644549	2.175580
14	1	0	-1.475372	-3.380047	-0.609713
15	1	0	-3.076612	-2.965012	-1.191023
16	1	0	-3.386092	-1.368418	0.678795
17	1	0	-3.072948	-3.016753	1.220022
18	1	0	-0.423816	-3.355339	1.198804
19	1	0	-1.084551	-3.263601	2.828209
20	1	0	0.539458	-1.391212	3.346625
21	1	0	1.277885	-2.963941	3.047030
22	1	0	1.475373	-3.380048	0.609714
23	1	0	3.076612	-2.965012	1.191024
24	1	0	3.386092	-1.368417	-0.678796
25	1	0	3.072948	-3.016752	-1.220021
26	1	0	0.423816	-3.355338	-1.198803
27	1	0	1.084551	-3.263599	-2.828208
28	1	0	-0.539458	-1.391213	-3.346626
29	1	0	-1.277884	-2.963942	-3.047030
30	1	0	-2.124426	-0.100562	-2.990344
31	1	0	-3.393202	-1.277307	-2.632786
32	1	0	2.124426	-0.100561	2.990344
33	1	0	3.393202	-1.277305	2.632785
34	6	0	-3.246232	0.384949	-1.253322
35	6	0	-4.556080	0.844764	-1.404228
36	6	0	-5.009643	1.865375	-0.558982
37	1	0	-5.205132	0.423112	-2.165626

38	6	0	-2.870749	1.856943	0.524120
39	6	0	-4.161064	2.379695	0.422418
40	1	0	-6.021727	2.244569	-0.663911
41	1	0	-4.463890	3.158173	1.113630
42	6	0	3.246232	0.384949	1.253322
43	6	0	4.556081	0.844763	1.404228
44	6	0	2.870749	1.856944	-0.524120
45	6	0	5.009643	1.865374	0.558982
46	1	0	5.205132	0.423113	2.165625
47	6	0	4.161064	2.379695	-0.422417
48	1	0	6.021727	2.244568	0.663910
49	1	0	4.463890	3.158173	-1.113630
50	7	0	2.434152	0.892271	0.309599
51	7	0	-2.434153	0.892271	-0.309599
52	6	0	-1.896002	2.301601	1.617080
53	8	0	-0.741569	1.680827	1.575511
54	8	0	-2.267437	3.136003	2.429317
55	6	0	1.896002	2.301602	-1.617078
56	8	0	2.267436	3.136004	-2.429317
57	8	0	0.741569	1.680827	-1.575510
58	7	0	1.512477	-1.593230	-1.568727
59	7	0	-1.512476	-1.593231	1.568726
60	6	0	-2.118931	-0.924119	2.748586
61	1	0	-1.353201	-0.428635	3.346154
62	1	0	-2.818284	-0.158544	2.411438
63	1	0	-2.658276	-1.651821	3.374501
64	6	0	2.118931	-0.924118	-2.748586
65	1	0	1.353201	-0.428635	-3.346154
66	1	0	2.818284	-0.158543	-2.411438
67	1	0	2.658276	-1.651820	-3.374501

E(RTPSSh) = -1596.97742835

Zero-point correction= 0.560013 (Hartree/Particle)

Thermal correction to Energy= 0.591393

Thermal correction to Enthalpy= 0.592337

Thermal correction to Gibbs Free Energy= 0.500773

Sum of electronic and zero-point Energies= -1596.423196

Sum of electronic and thermal Energies= -1596.391815

Sum of electronic and thermal Enthalpies= -1596.390871

Sum of electronic and thermal Free Energies= -1596.482436

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	0.000000	0.094125	0.000000
2	7	0	1.722134	-1.218114	-1.580270
3	6	0	0.926783	-1.859951	-2.667360
4	6	0	-0.226946	-2.746927	-2.188776
5	6	0	-1.872256	-2.909669	-0.365544
6	6	0	-2.562332	-2.174134	0.795523
7	7	0	-1.722134	-1.218114	1.580269
8	6	0	-0.926783	-1.859952	2.667359
9	6	0	0.226945	-2.746928	2.188775
10	6	0	1.872256	-2.909669	0.365543
11	6	0	2.562332	-2.174134	-0.795524
12	6	0	2.617681	-0.189135	-2.201171
13	6	0	-2.617681	-0.189136	2.201171
14	1	0	1.580889	-2.461657	-3.318913
15	1	0	0.520080	-1.044896	-3.274842
16	1	0	-1.116813	-3.600087	0.010826
17	1	0	-2.641335	-3.528012	-0.857622
18	1	0	-3.397552	-1.594923	0.391786
19	1	0	-2.997698	-2.930374	1.467623
20	1	0	-1.580889	-2.461658	3.318912
21	1	0	-0.520080	-1.044897	3.274841
22	1	0	1.116812	-3.600087	-0.010828
23	1	0	2.641334	-3.528013	0.857621
24	1	0	3.397551	-1.594923	-0.391786
25	1	0	2.997698	-2.930373	-1.467624
26	1	0	3.424373	-0.666498	-2.776924

27	1	0	2.006959	0.390500	-2.903526
28	1	0	-3.424373	-0.666500	2.776924
29	1	0	-2.006959	0.390499	2.903526
30	6	0	3.186648	0.764345	-1.166186
31	6	0	4.433809	1.382855	-1.274685
32	6	0	4.814335	2.299886	-0.286425
33	1	0	5.089961	1.160980	-2.110567
34	6	0	2.735984	1.893939	0.835498
35	6	0	3.960833	2.560704	0.787852
36	1	0	5.776839	2.798006	-0.354361
37	1	0	4.214125	3.250886	1.584699
38	6	0	-3.186648	0.764345	1.166186
39	6	0	-4.433809	1.382854	1.274685
40	6	0	-2.735984	1.893940	-0.835497
41	6	0	-4.814335	2.299885	0.286425
42	1	0	-5.089962	1.160977	2.110567
43	6	0	-3.960833	2.560705	-0.787852
44	1	0	-5.776839	2.798005	0.354361
45	1	0	-4.214125	3.250887	-1.584698
46	7	0	-2.371895	1.028181	0.129570
47	7	0	2.371895	1.028180	-0.129569
48	6	0	1.746257	2.063214	1.988946
49	8	0	0.637540	1.374923	1.836427
50	8	0	2.055831	2.773585	2.934117
51	6	0	-1.746257	2.063215	-1.988945
52	8	0	-2.055830	2.773587	-2.934115
53	8	0	-0.637539	1.374924	-1.836426
54	1	0	0.720330	-3.161097	3.080904
55	1	0	-0.151820	-3.602946	1.628286
56	1	0	0.151820	-3.602945	-1.628287
57	1	0	-0.720330	-3.161096	-3.080906
58	7	0	1.213913	-2.010640	1.346565
59	7	0	-1.213913	-2.010639	-1.346565
60	6	0	2.235495	-1.400781	2.237838
61	1	0	2.941148	-0.811700	1.650349
62	1	0	1.751800	-0.729835	2.949025

63	1	0	2.785647	-2.182234	2.783850
64	6	0	-2.235495	-1.400779	-2.237838
65	1	0	-2.941148	-0.811699	-1.650349
66	1	0	-1.751801	-0.729833	-2.949025
67	1	0	-2.785647	-2.182232	-2.783851

E(RTPSSh) = -1596.97290762

Zero-point correction= 0.559730 (Hartree/Particle)

Thermal correction to Energy= 0.591314

Thermal correction to Enthalpy= 0.592259

Thermal correction to Gibbs Free Energy= 0.499834

Sum of electronic and zero-point Energies= -1596.415543

Sum of electronic and thermal Energies= -1596.383959

Sum of electronic and thermal Enthalpies= -1596.383015

Sum of electronic and thermal Free Energies= -1596.475439

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.537747	-1.864741	0.973033
2	6	0	-0.734134	-2.741819	1.883138
3	6	0	0.272670	-1.979276	2.740354
4	6	0	2.400753	-1.946339	1.432839
5	6	0	2.105770	-2.699165	0.135706
6	7	0	1.537789	-1.864797	-0.972975
7	6	0	0.734197	-2.741925	-1.883051
8	6	0	-0.272623	-1.979437	-2.740294
9	6	0	-2.400707	-1.946497	-1.432782
10	6	0	-2.105711	-2.699159	-0.135620
11	6	0	-2.643186	-1.268619	1.780997
12	6	0	2.643213	-1.268674	-1.780956
13	1	0	-0.232610	-3.488296	1.270114
14	1	0	-1.398857	-3.298552	2.560240
15	1	0	3.221269	-1.246500	1.265603

16	1	0	2.754277	-2.683494	2.170928
17	1	0	3.043073	-3.169791	-0.193327
18	1	0	1.410664	-3.515742	0.323780
19	1	0	0.232691	-3.488393	-1.269999
20	1	0	1.398935	-3.298667	-2.560131
21	1	0	-3.221240	-1.246671	-1.265571
22	1	0	-2.754215	-2.683687	-2.170844
23	1	0	-3.043003	-3.169795	0.193428
24	1	0	-1.410587	-3.515728	-0.323665
25	1	0	-3.376241	-2.043528	2.044475
26	1	0	-2.211195	-0.908125	2.721197
27	1	0	3.376289	-2.043573	-2.044407
28	1	0	2.211215	-0.908224	-2.721171
29	6	0	-3.332833	-0.098218	1.119179
30	6	0	-4.683399	0.191221	1.338900
31	6	0	-5.224988	1.345413	0.768164
32	1	0	-5.291735	-0.470896	1.945992
33	6	0	-3.079462	1.805779	-0.200393
34	6	0	-4.412199	2.170363	-0.012301
35	1	0	-6.269662	1.592954	0.928232
36	1	0	-4.782896	3.075157	-0.479328
37	6	0	3.332830	-0.098230	-1.119180
38	6	0	4.683387	0.191237	-1.338916
39	6	0	3.079411	1.805809	0.200320
40	6	0	5.224947	1.345465	-0.768226
41	1	0	5.291739	-0.470886	-1.945986
42	6	0	4.412137	2.170421	0.012211
43	1	0	6.269614	1.593028	-0.928306
44	1	0	4.782810	3.075244	0.479204
45	7	0	2.559043	0.694770	-0.358047
46	7	0	-2.559066	0.694776	0.358018
47	6	0	-2.125283	2.626170	-1.057017
48	8	0	-0.940718	2.118442	-1.176168
49	8	0	-2.538057	3.675497	-1.567996
50	6	0	2.125213	2.626203	1.056917
51	8	0	2.537958	3.675562	1.567854

52	8	0	0.940662	2.118448	1.176092
53	1	0	-0.786132	-2.706239	-3.388544
54	1	0	0.262459	-1.292627	-3.403510
55	1	0	-0.262429	-1.292452	3.403542
56	1	0	0.786192	-2.706041	3.388633
57	7	0	-1.275291	-1.151235	-2.005979
58	7	0	1.275320	-1.151080	2.006008
59	6	0	-1.876231	-0.241427	-3.021514
60	1	0	-2.656926	0.359714	-2.554934
61	1	0	-1.108227	0.425030	-3.416928
62	1	0	-2.318118	-0.818677	-3.846955
63	6	0	1.876241	-0.241224	3.021510
64	1	0	2.656924	0.359916	2.554908
65	1	0	1.108225	0.425231	3.416902
66	1	0	2.318143	-0.818436	3.846972
67	60	0	0.000006	0.236714	0.000014

E(RTPSSh) = -1596.96846206

Zero-point correction= 0.561228 (Hartree/Particle)

Thermal correction to Energy= 0.592531

Thermal correction to Enthalpy= 0.593475

Thermal correction to Gibbs Free Energy= 0.501634

Sum of electronic and zero-point Energies= -1596.407286

Sum of electronic and thermal Energies= -1596.375983

Sum of electronic and thermal Enthalpies= -1596.375039

Sum of electronic and thermal Free Energies= -1596.466880

[Eu(Me$_2$dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000000	0.023395	0.000000

2	7	0	1.870783	-1.609401	-1.075191
3	6	0	1.271385	-2.648569	-1.957755
4	6	0	0.053646	-2.156068	-2.739142
5	6	0	-1.743106	-2.757424	-1.172592
6	6	0	-2.635130	-2.263288	-0.029712
7	7	0	-1.870783	-1.609401	1.075191
8	6	0	-1.271385	-2.648569	1.957755
9	6	0	-0.053646	-2.156068	2.739142
10	6	0	1.743106	-2.757424	1.172592
11	6	0	2.635130	-2.263288	0.029711
12	6	0	2.789634	-0.733622	-1.863738
13	6	0	-2.789634	-0.733623	1.863738
14	1	0	0.996095	-3.499372	-1.328251
15	1	0	2.020026	-3.025136	-2.671463
16	1	0	0.340931	-1.328025	-3.395170
17	1	0	-0.295348	-2.971845	-3.393386
18	1	0	-0.987172	-3.444660	-0.779235
19	1	0	-2.362925	-3.339724	-1.873908
20	1	0	-3.354353	-1.534385	-0.409368
21	1	0	-3.215165	-3.112049	0.363676
22	1	0	-0.996095	-3.499372	1.328251
23	1	0	-2.020026	-3.025136	2.671463
24	1	0	-0.340931	-1.328026	3.395170
25	1	0	0.295348	-2.971846	3.393386
26	1	0	0.987172	-3.444660	0.779235
27	1	0	2.362925	-3.339724	1.873908
28	1	0	3.354353	-1.534385	0.409368
29	1	0	3.215165	-3.112049	-0.363676
30	1	0	3.664196	-1.304473	-2.211237
31	1	0	2.246951	-0.396406	-2.754892
32	1	0	-3.664196	-1.304473	2.211236
33	1	0	-2.246952	-0.396406	2.754892
34	6	0	3.227692	0.480593	-1.064005
35	6	0	4.442338	1.140243	-1.256201
36	6	0	4.715599	2.275453	-0.482652
37	1	0	5.157011	0.781990	-1.990738

38	6	0	2.604729	1.986656	0.614381
39	6	0	3.791831	2.705576	0.471954
40	1	0	5.651056	2.809517	-0.619530
41	1	0	3.962371	3.566519	1.108379
42	6	0	-3.227692	0.480592	1.064005
43	6	0	-4.442339	1.140242	1.256201
44	6	0	-2.604729	1.986657	-0.614381
45	6	0	-4.715599	2.275453	0.482651
46	1	0	-5.157012	0.781990	1.990738
47	6	0	-3.791831	2.705576	-0.471954
48	1	0	-5.651056	2.809516	0.619530
49	1	0	-3.962371	3.566519	-1.108379
50	7	0	-2.341236	0.909329	0.149703
51	7	0	2.341237	0.909329	-0.149703
52	6	0	1.546068	2.330899	1.660742
53	8	0	0.487056	1.555849	1.604015
54	8	0	1.765335	3.237066	2.450418
55	6	0	-1.546068	2.330899	-1.660742
56	8	0	-1.765335	3.237066	-2.450417
57	8	0	-0.487056	1.555849	-1.604015
58	7	0	-1.053895	-1.652561	-1.883968
59	7	0	1.053895	-1.652561	1.883968
60	6	0	2.018428	-0.947809	2.768630
61	1	0	2.835007	-0.532873	2.176229
62	1	0	1.510233	-0.120394	3.264940
63	1	0	2.433478	-1.636340	3.520553
64	6	0	-2.018428	-0.947809	-2.768630
65	1	0	-2.835007	-0.532873	-2.176229
66	1	0	-1.510233	-0.120394	-3.264940
67	1	0	-2.433478	-1.636339	-3.520553

E(RTPSSh) = -1598.80105364

Zero-point correction= 0.559652 (Hartree/Particle)

Thermal correction to Energy= 0.591296

Thermal correction to Enthalpy= 0.592241

Thermal correction to Gibbs Free Energy= 0.499988

Sum of electronic and zero-point Energies= -1598.247304

Sum of electronic and thermal Energies= -1598.215659

Sum of electronic and thermal Enthalpies= -1598.214715

Sum of electronic and thermal Free Energies= -1598.306967

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000000	0.000000	0.086756
2	7	0	-1.338253	-1.698716	-1.505899
3	6	0	-0.449715	-2.228801	-2.587859
4	6	0	0.985847	-2.524223	-2.157886
5	6	0	2.108464	-0.407776	-2.667082
6	6	0	2.488935	0.974901	-2.136700
7	7	0	1.338253	1.698716	-1.505899
8	6	0	0.449715	2.228801	-2.587859
9	6	0	-0.985847	2.524223	-2.157886
10	6	0	-2.108464	0.407776	-2.667082
11	6	0	-2.488935	-0.974901	-2.136700
12	6	0	-1.875615	-2.823232	-0.682441
13	6	0	1.875615	2.823232	-0.682441
14	1	0	-0.444904	-1.496991	-3.398374
15	1	0	-0.884903	-3.148227	-3.003962
16	1	0	1.002383	-3.311501	-1.401745
17	1	0	1.531071	-2.909368	-3.033096
18	1	0	1.288717	-0.322892	-3.385052
19	1	0	2.966106	-0.821022	-3.218872
20	1	0	3.269115	0.878933	-1.378131
21	1	0	2.909111	1.569916	-2.959836
22	1	0	0.444904	1.496991	-3.398374
23	1	0	0.884903	3.148227	-3.003962
24	1	0	-1.002383	3.311501	-1.401745
25	1	0	-1.531071	2.909368	-3.033096
26	1	0	-1.288717	0.322892	-3.385052

27	1	0	-2.966106	0.821022	-3.218872
28	1	0	-3.269115	-0.878933	-1.378131
29	1	0	-2.909111	-1.569916	-2.959836
30	1	0	-2.750388	-2.442992	-0.142639
31	1	0	-2.221536	-3.644463	-1.324016
32	1	0	2.750388	2.442992	-0.142639
33	1	0	2.221536	3.644463	-1.324016
34	6	0	-0.896804	-3.332253	0.354192
35	6	0	-0.873593	-4.663376	0.784250
36	6	0	0.000000	-5.023243	1.813497
37	1	0	-1.523602	-5.398193	0.321347
38	6	0	0.761608	-2.752256	1.889164
39	6	0	0.828920	-4.053741	2.382675
40	1	0	0.036409	-6.050610	2.161769
41	1	0	1.524917	-4.281462	3.181402
42	6	0	0.896804	3.332253	0.354192
43	6	0	0.873593	4.663376	0.784250
44	6	0	-0.761608	2.752256	1.889164
45	6	0	0.000000	5.023243	1.813497
46	1	0	1.523602	5.398193	0.321347
47	6	0	-0.828920	4.053741	2.382675
48	1	0	-0.036409	6.050610	2.161769
49	1	0	-1.524917	4.281462	3.181402
50	7	0	0.084830	2.408790	0.898227
51	7	0	-0.084830	-2.408790	0.898227
52	6	0	1.649195	-1.636040	2.415197
53	8	0	1.525238	-0.509065	1.789529
54	8	0	2.396931	-1.866708	3.349608
55	6	0	-1.649195	1.636040	2.415197
56	8	0	-2.396931	1.866708	3.349608
57	8	0	-1.525238	0.509065	1.789529
58	7	0	-1.692281	1.344780	-1.586545
59	7	0	1.692281	-1.344780	-1.586545
60	6	0	-2.904552	1.827937	-0.877716
61	1	0	-3.415557	0.995537	-0.392059
62	1	0	-2.612044	2.546351	-0.110514

63	1	0	-3.596935	2.317359	-1.578364
64	6	0	2.904552	-1.827937	-0.877716
65	1	0	3.415557	-0.995537	-0.392059
66	1	0	2.612044	-2.546351	-0.110514
67	1	0	3.596935	-2.317359	-1.578364

E(RTPSSh) = -1598.80223844

Zero-point correction= 0.560641 (Hartree/Particle)

Thermal correction to Energy= 0.591941

Thermal correction to Enthalpy= 0.592885

Thermal correction to Gibbs Free Energy= 0.501735

Sum of electronic and zero-point Energies= -1598.242346

Sum of electronic and thermal Energies= -1598.211047

Sum of electronic and thermal Enthalpies= -1598.210103

Sum of electronic and thermal Free Energies= -1598.301253

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	63	0	0.000000	0.028507	0.000000
2	7	0	1.694671	-1.199113	-1.583996
3	6	0	0.896297	-1.838323	-2.670614
4	6	0	-0.247220	-2.733817	-2.183651
5	6	0	-1.882430	-2.897873	-0.346181
6	6	0	-2.555035	-2.154498	0.820355
7	7	0	-1.694670	-1.199114	1.583996
8	6	0	-0.896297	-1.838323	2.670614
9	6	0	0.247220	-2.733817	2.183651
10	6	0	1.882430	-2.897873	0.346181
11	6	0	2.555035	-2.154498	-0.820356
12	6	0	2.563427	-0.141736	-2.195434
13	6	0	-2.563427	-0.141736	2.195434
14	1	0	1.548802	-2.431643	-3.331030
15	1	0	0.478247	-1.020846	-3.266323

16	1	0	-1.127176	-3.592773	0.022781
17	1	0	-2.658868	-3.511098	-0.832406
18	1	0	-3.393003	-1.573133	0.425350
19	1	0	-2.984297	-2.903910	1.503491
20	1	0	-1.548802	-2.431643	3.331030
21	1	0	-0.478246	-1.020846	3.266323
22	1	0	1.127176	-3.592773	-0.022781
23	1	0	2.658868	-3.511097	0.832406
24	1	0	3.393003	-1.573133	-0.425350
25	1	0	2.984298	-2.903910	-1.503491
26	1	0	3.380682	-0.591433	-2.777967
27	1	0	1.933364	0.432757	-2.884196
28	1	0	-3.380682	-0.591433	2.777967
29	1	0	-1.933364	0.432757	2.884196
30	6	0	3.104323	0.814175	-1.148384
31	6	0	4.324646	1.485743	-1.248179
32	6	0	4.666761	2.404288	-0.247219
33	1	0	4.988573	1.303551	-2.087472
34	6	0	2.608259	1.898564	0.868793
35	6	0	3.803290	2.616800	0.830270
36	1	0	5.607710	2.942787	-0.308575
37	1	0	4.028082	3.307942	1.634801
38	6	0	-3.104323	0.814175	1.148384
39	6	0	-4.324646	1.485743	1.248179
40	6	0	-2.608260	1.898564	-0.868793
41	6	0	-4.666761	2.404288	0.247220
42	1	0	-4.988573	1.303552	2.087473
43	6	0	-3.803290	2.616799	-0.830270
44	1	0	-5.607711	2.942789	0.308575
45	1	0	-4.028082	3.307942	-1.634800
46	7	0	-2.282749	1.029567	0.106716
47	7	0	2.282749	1.029568	-0.106716
48	6	0	1.606226	2.008506	2.017347
49	8	0	0.529546	1.273098	1.847539
50	8	0	1.875788	2.718022	2.975201
51	6	0	-1.606227	2.008506	-2.017347

52	8	0	-1.875788	2.718022	-2.975201
53	8	0	-0.529546	1.273099	-1.847539
54	1	0	0.748767	-3.149248	3.070392
55	1	0	-0.139423	-3.588396	1.626259
56	1	0	0.139423	-3.588396	-1.626259
57	1	0	-0.748767	-3.149248	-3.070392
58	7	0	1.228239	-1.999289	1.331405
59	7	0	-1.228239	-1.999289	-1.331405
60	6	0	2.256526	-1.390579	2.216327
61	1	0	2.954525	-0.796836	1.625036
62	1	0	1.776219	-0.726063	2.935223
63	1	0	2.813100	-2.174244	2.752144
64	6	0	-2.256526	-1.390580	-2.216327
65	1	0	-2.954525	-0.796836	-1.625037
66	1	0	-1.776219	-0.726063	-2.935223
67	1	0	-2.813100	-2.174244	-2.752144

E(RTPSSh) = -1598.79515419

Zero-point correction= 0.560124 (Hartree/Particle)

Thermal correction to Energy= 0.591607

Thermal correction to Enthalpy= 0.592552

Thermal correction to Gibbs Free Energy= 0.500484

Sum of electronic and zero-point Energies= -1598.237210

Sum of electronic and thermal Energies= -1598.205726

Sum of electronic and thermal Enthalpies= -1598.204782

Sum of electronic and thermal Free Energies= -1598.296850

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.537616	-1.851599	0.997944
2	6	0	-0.746724	-2.750813	1.895432
3	6	0	0.283502	-2.023371	2.758763
4	6	0	2.398993	-1.927124	1.426417

5	6	0	2.116826	-2.669594	0.116928
6	7	0	1.537616	-1.851599	-0.997945
7	6	0	0.746724	-2.750813	-1.895432
8	6	0	-0.283502	-2.023372	-2.758763
9	6	0	-2.398993	-1.927124	-1.426417
10	6	0	-2.116826	-2.669594	-0.116928
11	6	0	-2.622565	-1.210468	1.808188
12	6	0	2.622565	-1.210468	-1.808188
13	1	0	-0.252573	-3.491054	1.265843
14	1	0	-1.416805	-3.313491	2.564250
15	1	0	3.195360	-1.199886	1.257935
16	1	0	2.790703	-2.670089	2.141940
17	1	0	3.063081	-3.127308	-0.209749
18	1	0	1.431492	-3.497968	0.302246
19	1	0	0.252573	-3.491053	-1.265842
20	1	0	1.416805	-3.313492	-2.564250
21	1	0	-3.195360	-1.199885	-1.257935
22	1	0	-2.790703	-2.670088	-2.141941
23	1	0	-3.063081	-3.127308	0.209749
24	1	0	-1.431493	-3.497967	-0.302246
25	1	0	-3.398467	-1.952614	2.049604
26	1	0	-2.177363	-0.898453	2.760558
27	1	0	3.398467	-1.952614	-2.049604
28	1	0	2.177362	-0.898454	-2.760558
29	6	0	-3.240035	0.011222	1.155261
30	6	0	-4.558233	0.412841	1.375880
31	6	0	-5.003653	1.600215	0.780384
32	1	0	-5.220679	-0.180165	1.999062
33	6	0	-2.845040	1.852358	-0.233274
34	6	0	-4.141857	2.330746	-0.039191
35	1	0	-6.022106	1.938454	0.946270
36	1	0	-4.440305	3.243143	-0.543155
37	6	0	3.240035	0.011222	-1.155261
38	6	0	4.558233	0.412841	-1.375880
39	6	0	2.845040	1.852357	0.233275
40	6	0	5.003653	1.600215	-0.780385

41	1	0	5.220679	-0.180165	-1.999063
42	6	0	4.141857	2.330746	0.039190
43	1	0	6.022105	1.938454	-0.946272
44	1	0	4.440305	3.243142	0.543154
45	7	0	2.413451	0.729270	-0.375607
46	7	0	-2.413451	0.729270	0.375607
47	6	0	-1.860675	2.514154	-1.200748
48	8	0	-0.733206	1.861514	-1.317566
49	8	0	-2.215572	3.521342	-1.796239
50	6	0	1.860676	2.514153	1.200747
51	8	0	2.215573	3.521341	1.796239
52	8	0	0.733207	1.861514	1.317567
53	1	0	-0.801697	-2.776432	-3.375621
54	1	0	0.235012	-1.359827	-3.458468
55	1	0	-0.235012	-1.359827	3.458468
56	1	0	0.801696	-2.776432	3.375620
57	7	0	-1.267238	-1.173103	-2.034914
58	7	0	1.267238	-1.173103	2.034914
59	6	0	-1.862628	-0.267730	-3.062159
60	1	0	-2.638240	0.345184	-2.604398
61	1	0	-1.095632	0.399691	-3.455899
62	1	0	-2.306530	-0.853331	-3.881377
63	6	0	1.862628	-0.267730	3.062159
64	1	0	2.638240	0.345184	2.604399
65	1	0	1.095632	0.399691	3.455900
66	1	0	2.306530	-0.853330	3.881377
67	63	0	0.000000	0.163959	0.000000

E(RTPSSh) = -1598.78127363

Zero-point correction= 0.561246 (Hartree/Particle)

Thermal correction to Energy= 0.592524

Thermal correction to Enthalpy= 0.593468

Thermal correction to Gibbs Free Energy= 0.501736

Sum of electronic and zero-point Energies= -1598.225496

Sum of electronic and thermal Energies= -1598.194219

Sum of electronic and thermal Enthalpies= -1598.193275

Sum of electronic and thermal Free Energies= -1598.285007

[Gd(Me$_2$dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.009121	0.000000
2	7	0	-1.865419	-1.605377	1.077622
3	6	0	-1.268159	-2.643391	1.962755
4	6	0	-0.047841	-2.150348	2.739240
5	6	0	1.744211	-2.754820	1.168089
6	6	0	2.633838	-2.260502	0.023646
7	7	0	1.865419	-1.605377	-1.077622
8	6	0	1.268158	-2.643390	-1.962755
9	6	0	0.047841	-2.150348	-2.739240
10	6	0	-1.744212	-2.754820	-1.168089
11	6	0	-2.633838	-2.260502	-0.023646
12	6	0	-2.779290	-0.722154	1.863850
13	6	0	2.779290	-0.722154	-1.863850
14	1	0	-0.996429	-3.497219	1.335742
15	1	0	-2.016547	-3.014985	2.679249
16	1	0	-0.332547	-1.320832	3.394403
17	1	0	0.303666	-2.964918	3.393525
18	1	0	0.987261	-3.441844	0.776180
19	1	0	2.364719	-3.336648	1.869091
20	1	0	3.354059	-1.531885	0.401948
21	1	0	3.212598	-3.108714	-0.372539
22	1	0	0.996428	-3.497219	-1.335742
23	1	0	2.016547	-3.014985	-2.679250
24	1	0	0.332547	-1.320833	-3.394403
25	1	0	-0.303667	-2.964918	-3.393526
26	1	0	-0.987262	-3.441844	-0.776181

27	1	0	-2.364720	-3.336647	-1.869090
28	1	0	-3.354059	-1.531885	-0.401948
29	1	0	-3.212598	-3.108714	0.372540
30	1	0	-3.657125	-1.286872	2.212883
31	1	0	-2.234406	-0.384550	2.753438
32	1	0	3.657124	-1.286872	-2.212884
33	1	0	2.234406	-0.384550	-2.753438
34	6	0	-3.208763	0.491918	1.059518
35	6	0	-4.417581	1.162985	1.248781
36	6	0	-4.680268	2.297854	0.471017
37	1	0	-5.135657	0.813903	1.984398
38	6	0	-2.571219	1.987150	-0.623185
39	6	0	-3.751859	2.717134	-0.484073
40	1	0	-5.611057	2.840617	0.605446
41	1	0	-3.914235	3.577886	-1.122877
42	6	0	3.208764	0.491917	-1.059518
43	6	0	4.417581	1.162985	-1.248781
44	6	0	2.571219	1.987150	0.623186
45	6	0	4.680268	2.297854	-0.471018
46	1	0	5.135657	0.813903	-1.984398
47	6	0	3.751859	2.717134	0.484073
48	1	0	5.611057	2.840617	-0.605447
49	1	0	3.914235	3.577886	1.122876
50	7	0	2.318698	0.909547	-0.143930
51	7	0	-2.318698	0.909548	0.143931
52	6	0	-1.506739	2.317688	-1.667591
53	8	0	-0.454921	1.533103	-1.604945
54	8	0	-1.714804	3.222670	-2.461693
55	6	0	1.506739	2.317687	1.667591
56	8	0	1.714804	3.222670	2.461693
57	8	0	0.454921	1.533103	1.604945
58	7	0	1.056656	-1.648494	1.878898
59	7	0	-1.056656	-1.648494	-1.878898
60	6	0	-2.023558	-0.942917	-2.760507
61	1	0	-2.839016	-0.529006	-2.166051
62	1	0	-1.516293	-0.115240	-3.257189

63	1	0	-2.439838	-1.631062	-3.512036
64	6	0	2.023558	-0.942917	2.760507
65	1	0	2.839016	-0.529006	2.166051
66	1	0	1.516293	-0.115240	3.257189
67	1	0	2.439838	-1.631063	3.512036

E(RTPSSh) = -1599.39170445

Zero-point correction= 0.559559 (Hartree/Particle)

Thermal correction to Energy= 0.591294

Thermal correction to Enthalpy= 0.592238

Thermal correction to Gibbs Free Energy= 0.499260

Sum of electronic and zero-point Energies= -1598.838414

Sum of electronic and thermal Energies= -1598.806679

Sum of electronic and thermal Enthalpies= -1598.805735

Sum of electronic and thermal Free Energies= -1598.898713

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.077647	0.000000
2	7	0	-1.562771	-1.486797	-1.504033
3	6	0	-2.193446	-2.557106	-0.672462
4	6	0	-2.609982	-2.136640	0.737156
5	6	0	-0.599409	-2.671352	2.039497
6	6	0	0.734922	-2.134901	2.568270
7	7	0	1.562771	-1.486797	1.504033
8	6	0	2.193446	-2.557106	0.672461
9	6	0	2.609982	-2.136640	-0.737156
10	6	0	0.599409	-2.671352	-2.039497
11	6	0	-0.734922	-2.134901	-2.568270
12	6	0	-2.599173	-0.615493	-2.143102
13	6	0	2.599173	-0.615493	2.143102
14	1	0	-1.481472	-3.384591	-0.609380
15	1	0	-3.079492	-2.954289	-1.191379

16	1	0	-3.378059	-1.362517	0.682865
17	1	0	-3.068803	-3.010170	1.229452
18	1	0	-0.424320	-3.368344	1.213531
19	1	0	-1.085280	-3.250735	2.841515
20	1	0	0.547631	-1.388059	3.343480
21	1	0	1.290597	-2.958728	3.041598
22	1	0	1.481472	-3.384591	0.609380
23	1	0	3.079492	-2.954289	1.191378
24	1	0	3.378059	-1.362517	-0.682865
25	1	0	3.068803	-3.010170	-1.229453
26	1	0	0.424320	-3.368344	-1.213531
27	1	0	1.085280	-3.250735	-2.841516
28	1	0	-0.547631	-1.388059	-3.343480
29	1	0	-1.290597	-2.958727	-3.041598
30	1	0	-2.107503	-0.086364	-2.968143
31	1	0	-3.402173	-1.227149	-2.580208
32	1	0	2.107503	-0.086365	2.968143
33	1	0	3.402173	-1.227150	2.580208
34	6	0	-3.172229	0.436859	-1.211144
35	6	0	-4.453000	0.973775	-1.357657
36	6	0	-4.842883	2.016808	-0.508508
37	1	0	-5.127247	0.595182	-2.119745
38	6	0	-2.706420	1.880792	0.569052
39	6	0	-3.962551	2.480266	0.471153
40	1	0	-5.830948	2.455607	-0.610145
41	1	0	-4.217074	3.276560	1.161493
42	6	0	3.172229	0.436859	1.211144
43	6	0	4.453000	0.973775	1.357657
44	6	0	2.706420	1.880792	-0.569052
45	6	0	4.842883	2.016808	0.508509
46	1	0	5.127247	0.595182	2.119746
47	6	0	3.962551	2.480266	-0.471152
48	1	0	5.830948	2.455607	0.610146
49	1	0	4.217074	3.276560	-1.161492
50	7	0	2.333148	0.890905	0.265411
51	7	0	-2.333149	0.890905	-0.265411

52	6	0	-1.693487	2.260933	1.649937
53	8	0	-0.580122	1.568412	1.589814
54	8	0	-1.997659	3.114452	2.469809
55	6	0	1.693487	2.260934	-1.649937
56	8	0	1.997659	3.114453	-2.469808
57	8	0	0.580122	1.568413	-1.589814
58	7	0	1.499136	-1.591570	-1.561317
59	7	0	-1.499136	-1.591570	1.561317
60	6	0	2.096841	-0.902516	-2.735025
61	1	0	1.325414	-0.406562	-3.324004
62	1	0	2.789568	-0.135177	-2.388321
63	1	0	2.642528	-1.618611	-3.368378
64	6	0	-2.096841	-0.902517	2.735025
65	1	0	-1.325414	-0.406562	3.324004
66	1	0	-2.789568	-0.135177	2.388321
67	1	0	-2.642528	-1.618611	3.368377

E(RTPSSh) = -1599.38721845

Zero-point correction= 0.560444 (Hartree/Particle)

Thermal correction to Energy= 0.591723

Thermal correction to Enthalpy= 0.592667

Thermal correction to Gibbs Free Energy= 0.501420

Sum of electronic and zero-point Energies= -1598.834453

Sum of electronic and thermal Energies= -1598.803174

Sum of electronic and thermal Enthalpies= -1598.802230

Sum of electronic and thermal Free Energies= -1598.893477

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	64	0	0.000000	0.009601	0.000000
2	7	0	1.691672	-1.195598	-1.580474
3	6	0	0.896477	-1.836040	-2.668678
4	6	0	-0.246552	-2.732308	-2.182113

5	6	0	-1.885258	-2.894976	-0.346737
6	6	0	-2.556133	-2.149139	0.819132
7	7	0	-1.691673	-1.195599	1.580473
8	6	0	-0.896478	-1.836042	2.668677
9	6	0	0.246551	-2.732310	2.182112
10	6	0	1.885257	-2.894976	0.346735
11	6	0	2.556132	-2.149139	-0.819133
12	6	0	2.554771	-0.131430	-2.188122
13	6	0	-2.554771	-0.131431	2.188122
14	1	0	1.550803	-2.428798	-3.327674
15	1	0	0.478189	-1.019100	-3.264692
16	1	0	-1.131992	-3.591862	0.022687
17	1	0	-2.662605	-3.505903	-0.834188
18	1	0	-3.392571	-1.565717	0.423846
19	1	0	-2.987125	-2.896428	1.503388
20	1	0	-1.550804	-2.428799	3.327673
21	1	0	-0.478189	-1.019102	3.264691
22	1	0	1.131991	-3.591862	-0.022689
23	1	0	2.662604	-3.505904	0.834186
24	1	0	3.392570	-1.565718	-0.423847
25	1	0	2.987124	-2.896427	-1.503389
26	1	0	3.377166	-0.574469	-2.768378
27	1	0	1.921864	0.439756	-2.876786
28	1	0	-3.377167	-0.574470	2.768377
29	1	0	-1.921865	0.439755	2.876786
30	6	0	3.083680	0.827354	-1.137818
31	6	0	4.295527	1.514799	-1.233265
32	6	0	4.623290	2.435808	-0.229786
33	1	0	4.963641	1.342974	-2.071414
34	6	0	2.568834	1.902043	0.879962
35	6	0	3.754294	2.635867	0.845769
36	1	0	5.557381	2.986466	-0.287952
37	1	0	3.967985	3.329035	1.651582
38	6	0	-3.083680	0.827354	1.137818
39	6	0	-4.295527	1.514799	1.233265
40	6	0	-2.568834	1.902045	-0.879961

41	6	0	-4.623290	2.435809	0.229787
42	1	0	-4.963642	1.342973	2.071414
43	6	0	-3.754294	2.635869	-0.845768
44	1	0	-5.557380	2.986467	0.287952
45	1	0	-3.967984	3.329037	-1.651581
46	7	0	-2.257546	1.030050	0.097426
47	7	0	2.257546	1.030049	-0.097426
48	6	0	1.560341	1.996933	2.023721
49	8	0	0.494546	1.247105	1.847652
50	8	0	1.814719	2.708696	2.984104
51	6	0	-1.560340	1.996935	-2.023720
52	8	0	-1.814718	2.708698	-2.984102
53	8	0	-0.494545	1.247106	-1.847651
54	1	0	0.747959	-3.148551	3.068488
55	1	0	-0.139933	-3.586203	1.623547
56	1	0	0.139932	-3.586202	-1.623549
57	1	0	-0.747960	-3.148549	-3.068490
58	7	0	1.227939	-1.996936	1.330680
59	7	0	-1.227939	-1.996935	-1.330681
60	6	0	2.254400	-1.387274	2.217275
61	1	0	2.952708	-0.792919	1.627082
62	1	0	1.772077	-0.723625	2.935497
63	1	0	2.810701	-2.170752	2.753515
64	6	0	-2.254400	-1.387273	-2.217275
65	1	0	-2.952708	-0.792918	-1.627082
66	1	0	-1.772077	-0.723622	-2.935497
67	1	0	-2.810702	-2.170750	-2.753516

E(RTPSSh) = -1599.38592822

Zero-point correction= 0.560360 (Hartree/Particle)

Thermal correction to Energy= 0.591697

Thermal correction to Enthalpy= 0.592642

Thermal correction to Gibbs Free Energy= 0.501410

Sum of electronic and zero-point Energies= -1598.827694

Sum of electronic and thermal Energies= -1598.796356

Sum of electronic and thermal Enthalpies= -1598.795412

Sum of electronic and thermal Free Energies= -1598.886643

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.571809	-1.871570	0.898851
2	6	0	-0.805646	-2.771427	1.819051
3	6	0	0.157289	-2.047303	2.713661
4	6	0	2.332804	-1.929614	1.522046
5	6	0	2.125704	-2.699289	0.221333
6	7	0	1.571795	-1.871587	-0.898837
7	6	0	0.805627	-2.771445	-1.819031
8	6	0	-0.157304	-2.047322	-2.713649
9	6	0	-2.332819	-1.929616	-1.522034
10	6	0	-2.125723	-2.699281	-0.221312
11	6	0	-2.670264	-1.223076	1.666733
12	6	0	2.670253	-1.223113	-1.666726
13	1	0	-0.286300	-3.503340	1.206413
14	1	0	-1.488993	-3.335422	2.454197
15	1	0	3.126331	-1.195006	1.378917
16	1	0	2.683673	-2.644109	2.276588
17	1	0	3.089287	-3.140555	-0.076044
18	1	0	1.447844	-3.536553	0.373767
19	1	0	0.286275	-3.503352	-1.206387
20	1	0	1.488971	-3.335450	-2.454173
21	1	0	-3.126343	-1.195006	-1.378908
22	1	0	-2.683692	-2.644115	-2.276570
23	1	0	-3.089307	-3.140540	0.076066
24	1	0	-1.447866	-3.536551	-0.373738
25	1	0	-3.461588	-1.960169	1.882304
26	1	0	-2.239364	-0.915084	2.627348
27	1	0	3.461573	-1.960213	-1.882291
28	1	0	2.239354	-0.915126	-2.627345
29	6	0	-3.267320	-0.000718	1.045172

30	6	0	-4.602488	0.361899	1.233034
31	6	0	-5.053231	1.554331	0.675442
32	1	0	-5.262619	-0.280808	1.802018
33	6	0	-2.856397	1.885870	-0.231510
34	6	0	-4.168278	2.334770	-0.074431
35	1	0	-6.084982	1.862277	0.810278
36	1	0	-4.472368	3.261897	-0.543936
37	6	0	3.267324	-0.000749	-1.045177
38	6	0	4.602507	0.361864	-1.233041
39	6	0	2.856417	1.885863	0.231496
40	6	0	5.053256	1.554298	-0.675456
41	1	0	5.262632	-0.280852	-1.802019
42	6	0	4.168310	2.334752	0.074409
43	1	0	6.085007	1.862235	-0.810293
44	1	0	4.472405	3.261880	0.543907
45	7	0	2.421384	0.755193	-0.337009
46	7	0	-2.421386	0.755207	0.337005
47	6	0	-1.837368	2.605888	-1.087528
48	8	0	-0.710176	1.968981	-1.246259
49	8	0	-2.143562	3.704027	-1.564249
50	6	0	1.837382	2.605902	1.087516
51	8	0	2.143594	3.704060	1.564233
52	8	0	0.710177	1.968990	1.246248
53	1	0	-0.671867	-2.788156	-3.346019
54	1	0	0.415201	-1.401816	-3.391276
55	1	0	-0.415212	-1.401787	3.391284
56	1	0	0.671849	-2.788135	3.346038
57	7	0	-1.157805	-1.179627	-2.041635
58	7	0	1.157795	-1.179618	2.041642
59	6	0	-1.656927	-0.246821	-3.077793
60	1	0	-2.436044	0.398891	-2.656437
61	1	0	-0.804131	0.377864	-3.409807
62	1	0	-2.078371	-0.803247	-3.927316
63	6	0	1.656922	-0.246807	3.077794
64	1	0	2.436043	0.398902	2.656434
65	1	0	0.804127	0.377885	3.409804

66	1	0	2.078363	-0.803227	3.927322
67	64	0	-0.000002	0.104519	0.000000

E(RTPSSh) = -1599.37374297

Zero-point correction= 0.560980 (Hartree/Particle)

Thermal correction to Energy= 0.592315

Thermal correction to Enthalpy= 0.593259

Thermal correction to Gibbs Free Energy= 0.501035

Sum of electronic and zero-point Energies= -1598.816781

Sum of electronic and thermal Energies= -1598.785446

Sum of electronic and thermal Enthalpies= -1598.784502

Sum of electronic and thermal Free Energies= -1598.876726

[Ho(Me_2dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000135	-0.053756	-0.000556
2	7	0	1.918713	-1.642754	-0.953619
3	6	0	1.355928	-2.688249	-1.854252
4	6	0	0.210835	-2.162693	-2.713727
5	6	0	-1.692390	-2.754190	-1.293047
6	6	0	-2.635380	-2.282514	-0.191074
7	7	0	-1.917181	-1.643314	0.954042
8	6	0	-1.353547	-2.687909	1.855217
9	6	0	-0.208832	-2.160992	2.714369
10	6	0	1.694725	-2.752490	1.294028
11	6	0	2.637432	-2.280834	0.191779
12	6	0	2.887737	-0.804594	-1.711753
13	6	0	-2.887194	-0.805982	1.711834
14	1	0	1.020414	-3.521332	-1.232738
15	1	0	2.141001	-3.088512	-2.511193

16	1	0	0.561533	-1.342183	-3.346983
17	1	0	-0.127426	-2.965391	-3.386056
18	1	0	-0.976239	-3.471185	-0.885273
19	1	0	-2.277091	-3.288281	-2.056824
20	1	0	-3.341530	-1.550510	-0.590174
21	1	0	-3.227263	-3.136122	0.167560
22	1	0	-1.017460	-3.521117	1.234190
23	1	0	-2.138307	-3.088342	2.512424
24	1	0	-0.560055	-1.340094	3.346835
25	1	0	0.129732	-2.962923	3.387467
26	1	0	0.978958	-3.470080	0.886616
27	1	0	2.279727	-3.285888	2.058067
28	1	0	3.343122	-1.548163	0.590465
29	1	0	3.229845	-3.134261	-0.166409
30	1	0	3.788938	-1.381305	-1.961531
31	1	0	2.419869	-0.508844	-2.656964
32	1	0	-3.787816	-1.383594	1.961607
33	1	0	-2.419780	-0.509500	2.657044
34	6	0	3.251944	0.442206	-0.937346
35	6	0	4.479596	1.096358	-1.077875
36	6	0	4.705433	2.265923	-0.348724
37	1	0	5.238868	0.694887	-1.740571
38	6	0	2.518861	2.030764	0.604049
39	6	0	3.711183	2.744563	0.508487
40	1	0	5.650827	2.790992	-0.441740
41	1	0	3.840621	3.642270	1.101466
42	6	0	-3.252559	0.440262	0.937131
43	6	0	-4.480973	1.093069	1.077364
44	6	0	-2.520956	2.029511	-0.604092
45	6	0	-4.708060	2.262246	0.347998
46	1	0	-5.239891	0.690838	1.740001
47	6	0	-3.714138	2.741914	-0.508992
48	1	0	-5.654089	2.786223	0.440697
49	1	0	-3.844411	3.639393	-1.102136
50	7	0	-2.302486	0.906361	0.108623
51	7	0	2.301590	0.907390	-0.108659

52	6	0	1.381503	2.448690	1.519327
53	8	0	0.354426	1.652406	1.488922
54	8	0	1.501134	3.468062	2.206430
55	6	0	-1.383786	2.448993	-1.518748
56	8	0	-1.504502	3.467927	-2.206305
57	8	0	-0.355475	1.654409	-1.487202
58	7	0	-0.935755	-1.634977	-1.918285
59	7	0	0.937562	-1.633331	1.918652
60	6	0	1.827440	-0.889811	2.847695
61	1	0	2.672406	-0.469607	2.300175
62	1	0	1.266623	-0.069731	3.297842
63	1	0	2.206113	-1.554061	3.637804
64	6	0	-1.825977	-0.892311	-2.847699
65	1	0	-2.671205	-0.472338	-2.300404
66	1	0	-1.265556	-0.072136	-3.298200
67	1	0	-2.204257	-1.557067	-3.637564

E(RTPSSh) = -1601.15677752

Zero-point correction= 0.559670 (Hartree/Particle)

Thermal correction to Energy= 0.591460

Thermal correction to Enthalpy= 0.592404

Thermal correction to Gibbs Free Energy= 0.499496

Sum of electronic and zero-point Energies= -1600.597106

Sum of electronic and thermal Energies= -1600.565317

Sum of electronic and thermal Enthalpies= -1600.564373

Sum of electronic and thermal Free Energies= -1600.657281

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000000	0.029280	0.000000
2	7	0	-1.544740	-1.475233	-1.503306
3	6	0	-2.193866	-2.546279	-0.687097
4	6	0	-2.614650	-2.128467	0.721216

5	6	0	-0.609504	-2.666055	2.033033
6	6	0	0.719227	-2.124036	2.568609
7	7	0	1.544739	-1.475232	1.503307
8	6	0	2.193865	-2.546279	0.687099
9	6	0	2.614648	-2.128469	-0.721215
10	6	0	0.609503	-2.666057	-2.033031
11	6	0	-0.719229	-2.124039	-2.568607
12	6	0	-2.564731	-0.581023	-2.137772
13	6	0	2.564731	-0.581022	2.137772
14	1	0	-1.490725	-3.381449	-0.624608
15	1	0	-3.079768	-2.929438	-1.216356
16	1	0	-3.381173	-1.352746	0.665606
17	1	0	-3.075697	-3.000910	1.212854
18	1	0	-0.427866	-3.363897	1.208996
19	1	0	-1.101938	-3.243763	2.832035
20	1	0	0.524934	-1.375174	3.339695
21	1	0	1.278037	-2.943169	3.045849
22	1	0	1.490723	-3.381448	0.624611
23	1	0	3.079767	-2.929438	1.216358
24	1	0	3.381173	-1.352749	-0.665606
25	1	0	3.075695	-3.000913	-1.212851
26	1	0	0.427865	-3.363900	-1.208994
27	1	0	1.101937	-3.243766	-2.832033
28	1	0	-0.524936	-1.375179	-3.339695
29	1	0	-1.278038	-2.943174	-3.045846
30	1	0	-2.061207	-0.054383	-2.956926
31	1	0	-3.379092	-1.174673	-2.578286
32	1	0	2.061207	-0.054381	2.956926
33	1	0	3.379092	-1.174673	2.578287
34	6	0	-3.113164	0.476641	-1.197889
35	6	0	-4.374202	1.058523	-1.343716
36	6	0	-4.730862	2.105857	-0.485391
37	1	0	-5.058001	0.711764	-2.112357
38	6	0	-2.604486	1.888190	0.597382
39	6	0	-3.838590	2.531393	0.501292
40	1	0	-5.703030	2.579049	-0.586021

41	1	0	-4.068689	3.330948	1.196400
42	6	0	3.113164	0.476641	1.197888
43	6	0	4.374203	1.058523	1.343715
44	6	0	2.604487	1.888189	-0.597384
45	6	0	4.730864	2.105856	0.485389
46	1	0	5.058002	0.711763	2.112357
47	6	0	3.838592	2.531392	-0.501294
48	1	0	5.703031	2.579047	0.586019
49	1	0	4.068691	3.330947	-1.196402
50	7	0	2.265176	0.892404	0.243767
51	7	0	-2.265176	0.892405	-0.243768
52	6	0	-1.575149	2.219115	1.677497
53	8	0	-0.485842	1.488986	1.599884
54	8	0	-1.842726	3.070810	2.511593
55	6	0	1.575150	2.219114	-1.677498
56	8	0	1.842727	3.070808	-2.511595
57	8	0	0.485842	1.488986	-1.599884
58	7	0	1.503463	-1.584810	-1.546391
59	7	0	-1.503464	-1.584808	1.546392
60	6	0	2.104587	-0.893119	-2.717406
61	1	0	1.334584	-0.400113	-3.310088
62	1	0	2.793483	-0.124018	-2.367193
63	1	0	2.656256	-1.608213	-3.346464
64	6	0	-2.104587	-0.893115	2.717406
65	1	0	-1.334585	-0.400110	3.310088
66	1	0	-2.793483	-0.124014	2.367193
67	1	0	-2.656257	-1.608209	3.346464

E(RTPSSh) = -1601.14903057

Zero-point correction= 0.561090 (Hartree/Particle)

Thermal correction to Energy= 0.592063

Thermal correction to Enthalpy= 0.593008

Thermal correction to Gibbs Free Energy= 0.502862

Sum of electronic and zero-point Energies= -1600.593343

Sum of electronic and thermal Energies= -1600.562369

Sum of electronic and thermal Enthalpies= -1600.561425

Sum of electronic and thermal Free Energies= -1600.651571

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	67	0	0.000000	0.034449	0.000000
2	7	0	-1.680003	1.182951	-1.571215
3	6	0	-0.893224	1.824554	-2.664569
4	6	0	0.247624	2.722825	-2.179171
5	6	0	1.889089	2.884242	-0.346117
6	6	0	2.555150	2.133808	0.818437
7	7	0	1.680003	1.182952	1.571216
8	6	0	0.893223	1.824553	2.664569
9	6	0	-0.247625	2.722823	2.179172
10	6	0	-1.889090	2.884242	0.346117
11	6	0	-2.555151	2.133808	-0.818437
12	6	0	-2.531948	0.105041	-2.169910
13	6	0	2.531948	0.105040	2.169910
14	1	0	-1.552220	2.414637	-3.321021
15	1	0	-0.474161	1.007883	-3.259496
16	1	0	1.138455	3.584174	0.023235
17	1	0	2.667402	3.491344	-0.836231
18	1	0	3.389564	1.546980	0.423792
19	1	0	2.987866	2.875755	1.507095
20	1	0	1.552219	2.414638	3.321021
21	1	0	0.474161	1.007883	3.259495
22	1	0	-1.138457	3.584174	-0.023234
23	1	0	-2.667404	3.491342	0.836232
24	1	0	-3.389564	1.546978	-0.423792
25	1	0	-2.987866	2.875754	-1.507094
26	1	0	-3.367829	0.534650	-2.740611
27	1	0	-1.895664	-0.457155	-2.862003
28	1	0	3.367829	0.534651	2.740612
29	1	0	1.895665	-0.457155	2.862003

30	6	0	-3.029417	-0.860388	-1.111791
31	6	0	-4.219995	-1.585637	-1.195440
32	6	0	-4.513057	-2.510632	-0.185276
33	1	0	-4.897936	-1.439444	-2.030522
34	6	0	-2.469381	-1.908376	0.907219
35	6	0	-3.631017	-2.678808	0.885290
36	1	0	-5.430222	-3.089857	-0.234539
37	1	0	-3.817546	-3.374652	1.695520
38	6	0	3.029417	-0.860388	1.111791
39	6	0	4.219995	-1.585636	1.195440
40	6	0	2.469381	-1.908375	-0.907218
41	6	0	4.513058	-2.510632	0.185276
42	1	0	4.897937	-1.439443	2.030522
43	6	0	3.631018	-2.678807	-0.885290
44	1	0	5.430223	-3.089856	0.234539
45	1	0	3.817547	-3.374651	-1.695521
46	7	0	2.191961	-1.030745	0.075173
47	7	0	-2.191961	-1.030745	-0.075174
48	6	0	-1.446565	-1.962872	2.038424
49	8	0	-0.409004	-1.178174	1.841435
50	8	0	-1.661987	-2.674579	3.008128
51	6	0	1.446566	-1.962873	-2.038425
52	8	0	1.661988	-2.674579	-3.008128
53	8	0	0.409004	-1.178174	-1.841435
54	1	0	-0.750953	3.139582	3.064012
55	1	0	0.138833	3.576147	1.619614
56	1	0	-0.138835	3.576147	-1.619613
57	1	0	0.750952	3.139583	-3.064010
58	7	0	-1.227341	1.984969	1.326843
59	7	0	1.227341	1.984970	-1.326842
60	6	0	-2.252864	1.376150	2.215997
61	1	0	-2.952671	0.781870	1.628015
62	1	0	-1.769067	0.714866	2.935060
63	1	0	-2.807406	2.161518	2.750967
64	6	0	2.252864	1.376153	-2.215997
65	1	0	2.952672	0.781872	-1.628015

66	1	0	1.769067	0.714867	-2.935060
67	1	0	2.807405	2.161520	-2.750967

E(RTPSSh) = -1601.14960747

Zero-point correction= 0.560641 (Hartree/Particle)

Thermal correction to Energy= 0.591930

Thermal correction to Enthalpy= 0.592875

Thermal correction to Gibbs Free Energy= 0.501791

Sum of electronic and zero-point Energies= -1600.590933

Sum of electronic and thermal Energies= -1600.559643

Sum of electronic and thermal Enthalpies= -1600.558699

Sum of electronic and thermal Free Energies= -1600.649782

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.519834	-1.850406	1.008252
2	6	0	-0.741148	-2.735587	1.931299
3	6	0	0.298589	-1.991500	2.766208
4	6	0	2.396818	-1.956851	1.402121
5	6	0	2.088858	-2.689788	0.094574
6	7	0	1.519834	-1.850406	-1.008252
7	6	0	0.741148	-2.735587	-1.931299
8	6	0	-0.298589	-1.991500	-2.766208
9	6	0	-2.396818	-1.956851	-1.402121
10	6	0	-2.088858	-2.689788	-0.094574
11	6	0	-2.609727	-1.186913	1.795460
12	6	0	2.609727	-1.186913	-1.795460
13	1	0	-0.257779	-3.501583	1.324310
14	1	0	-1.418235	-3.267748	2.617179
15	1	0	3.211566	-1.250569	1.230081
16	1	0	2.771439	-2.707250	2.118491
17	1	0	3.019649	-3.170593	-0.243398
18	1	0	1.381806	-3.499271	0.281684

19	1	0	0.257779	-3.501583	-1.324310
20	1	0	1.418235	-3.267748	-2.617179
21	1	0	-3.211566	-1.250569	-1.230081
22	1	0	-2.771439	-2.707251	-2.118491
23	1	0	-3.019649	-3.170593	0.243398
24	1	0	-1.381806	-3.499271	-0.281684
25	1	0	-3.407483	-1.911949	2.015504
26	1	0	-2.179200	-0.888620	2.758754
27	1	0	3.407483	-1.911949	-2.015504
28	1	0	2.179200	-0.888620	-2.758754
29	6	0	-3.179535	0.053967	1.134601
30	6	0	-4.478262	0.515586	1.354064
31	6	0	-4.869031	1.719592	0.753781
32	1	0	-5.166592	-0.043684	1.980299
33	6	0	-2.701891	1.872661	-0.260046
34	6	0	-3.975142	2.409623	-0.067221
35	1	0	-5.871197	2.103942	0.918469
36	1	0	-4.232419	3.334356	-0.571365
37	6	0	3.179535	0.053967	-1.134601
38	6	0	4.478262	0.515586	-1.354064
39	6	0	2.701891	1.872661	0.260046
40	6	0	4.869031	1.719592	-0.753780
41	1	0	5.166592	-0.043684	-1.980299
42	6	0	3.975142	2.409623	0.067221
43	1	0	5.871197	2.103942	-0.918468
44	1	0	4.232419	3.334356	0.571365
45	7	0	2.324759	0.731036	-0.350336
46	7	0	-2.324759	0.731036	0.350336
47	6	0	-1.682387	2.483039	-1.223748
48	8	0	-0.589342	1.772241	-1.338714
49	8	0	-1.981059	3.507612	-1.820044
50	6	0	1.682387	2.483039	1.223748
51	8	0	1.981059	3.507612	1.820044
52	8	0	0.589342	1.772241	1.338714
53	1	0	-0.815431	-2.727251	-3.404451
54	1	0	0.210308	-1.299166	-3.444683

55	1	0	-0.210308	-1.299166	3.444683
56	1	0	0.815431	-2.727251	3.404451
57	7	0	-1.283614	-1.173249	-2.006910
58	7	0	1.283614	-1.173249	2.006910
59	6	0	-1.905595	-0.256837	-3.008730
60	1	0	-2.677499	0.342034	-2.526214
61	1	0	-1.150873	0.421075	-3.406889
62	1	0	-2.362379	-0.834962	-3.826088
63	6	0	1.905595	-0.256837	3.008730
64	1	0	2.677499	0.342034	2.526214
65	1	0	1.150873	0.421076	3.406889
66	1	0	2.362379	-0.834962	3.826088
67	67	0	0.000000	0.098173	0.000000

E(RTPSSh) = -1601.13285992

Zero-point correction= 0.562119 (Hartree/Particle)

Thermal correction to Energy= 0.592928

Thermal correction to Enthalpy= 0.593872

Thermal correction to Gibbs Free Energy= 0.503805

Sum of electronic and zero-point Energies= -1600.575232

Sum of electronic and thermal Energies= -1600.544423

Sum of electronic and thermal Enthalpies= -1600.543479

Sum of electronic and thermal Free Energies= -1600.633546

[Yb(Me_2dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	0.000000	0.060379	0.000000
2	7	0	1.819318	1.569198	1.113504
3	6	0	1.224051	2.594351	2.014112
4	6	0	-0.021721	2.095740	2.740386

5	6	0	-1.755994	2.736430	1.113280
6	6	0	-2.621933	2.242617	-0.047935
7	7	0	-1.819318	1.569198	-1.113504
8	6	0	-1.224051	2.594351	-2.014112
9	6	0	0.021721	2.095740	-2.740386
10	6	0	1.755994	2.736430	-1.113281
11	6	0	2.621933	2.242617	0.047935
12	6	0	2.699225	0.641631	1.889476
13	6	0	-2.699225	0.641631	-1.889476
14	1	0	0.984453	3.471407	1.405959
15	1	0	1.961305	2.928518	2.759481
16	1	0	0.237112	1.248623	3.382956
17	1	0	-0.392691	2.897307	3.399428
18	1	0	-0.980579	3.410209	0.733654
19	1	0	-2.381361	3.327592	1.801494
20	1	0	-3.358928	1.523902	0.316449
21	1	0	-3.180619	3.089496	-0.473076
22	1	0	-0.984453	3.471407	-1.405959
23	1	0	-1.961305	2.928518	-2.759481
24	1	0	-0.237112	1.248623	-3.382956
25	1	0	0.392691	2.897307	-3.399428
26	1	0	0.980579	3.410209	-0.733654
27	1	0	2.381360	3.327592	-1.801494
28	1	0	3.358928	1.523902	-0.316449
29	1	0	3.180619	3.089496	0.473075
30	1	0	3.589148	1.172168	2.259716
31	1	0	2.133911	0.294256	2.761924
32	1	0	-3.589148	1.172168	-2.259716
33	1	0	-2.133911	0.294256	-2.761924
34	6	0	3.093002	-0.562502	1.053904
35	6	0	4.264165	-1.299660	1.235003
36	6	0	4.478031	-2.422088	0.424674
37	1	0	4.989187	-1.011353	1.989774
38	6	0	2.397667	-1.977184	-0.675557
39	6	0	3.538784	-2.768543	-0.549789
40	1	0	5.379110	-3.014545	0.551405

41	1	0	3.664705	-3.619675	-1.209351
42	6	0	-3.093002	-0.562502	-1.053904
43	6	0	-4.264165	-1.299660	-1.235004
44	6	0	-2.397667	-1.977184	0.675557
45	6	0	-4.478031	-2.422088	-0.424674
46	1	0	-4.989187	-1.011353	-1.989774
47	6	0	-3.538784	-2.768543	0.549789
48	1	0	-5.379109	-3.014545	-0.551406
49	1	0	-3.664705	-3.619675	1.209351
50	7	0	-2.197298	-0.907674	-0.116192
51	7	0	2.197298	-0.907674	0.116192
52	6	0	1.314730	-2.219273	-1.721887
53	8	0	0.298479	-1.391066	-1.616570
54	8	0	1.471799	-3.098857	-2.555356
55	6	0	-1.314730	-2.219273	1.721888
56	8	0	-1.471799	-3.098856	2.555357
57	8	0	-0.298479	-1.391066	1.616570
58	7	0	-1.099954	1.616713	1.833056
59	7	0	1.099954	1.616713	-1.833056
60	6	0	2.100312	0.923141	-2.687430
61	1	0	2.906262	0.519743	-2.074951
62	1	0	1.614733	0.093454	-3.201336
63	1	0	2.525606	1.619397	-3.426067
64	6	0	-2.100312	0.923141	2.687430
65	1	0	-2.906262	0.519743	2.074951
66	1	0	-1.614733	0.093455	3.201336
67	1	0	-2.525606	1.619397	3.426067

E(RTPSSh) = -1602.89981520

Zero-point correction= 0.560927 (Hartree/Particle)

Thermal correction to Energy= 0.591908

Thermal correction to Enthalpy= 0.592852

Thermal correction to Gibbs Free Energy= 0.503100

Sum of electronic and zero-point Energies= -1602.343427

Sum of electronic and thermal Energies= -1602.312446

Sum of electronic and thermal Enthalpies= -1602.311502

Sum of electronic and thermal Free Energies= -1602.401254

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	0.001922	-0.033232	-0.009138
2	7	0	1.581070	-1.509000	1.441879
3	6	0	2.155410	-2.596450	0.588316
4	6	0	2.550426	-2.156047	-0.816863
5	6	0	0.528749	-2.682136	-2.096807
6	6	0	-0.835177	-2.163971	-2.548447
7	7	0	-1.598017	-1.511888	-1.435223
8	6	0	-2.183055	-2.581597	-0.567430
9	6	0	-2.573114	-2.120090	0.832564
10	6	0	-0.556614	-2.650277	2.116002
11	6	0	0.811270	-2.140108	2.562502
12	6	0	2.670422	-0.666710	2.017704
13	6	0	-2.677652	-0.661651	-2.017812
14	1	0	1.412745	-3.394688	0.527981
15	1	0	3.036363	-3.027105	1.084375
16	1	0	3.328716	-1.391092	-0.771310
17	1	0	2.980959	-3.020963	-1.343108
18	1	0	0.411356	-3.426732	-1.305941
19	1	0	1.008703	-3.195217	-2.942968
20	1	0	-0.707015	-1.422133	-3.339829
21	1	0	-1.414361	-2.994986	-2.973869
22	1	0	-1.449252	-3.387285	-0.497869
23	1	0	-3.069272	-3.008738	-1.057289
24	1	0	-3.344202	-1.348609	0.777235
25	1	0	-3.012190	-2.974929	1.368321
26	1	0	-0.446075	-3.403058	1.331961
27	1	0	-1.039787	-3.152772	2.966833
28	1	0	0.689354	-1.387292	3.344452
29	1	0	1.382630	-2.971053	2.998507

30	1	0	2.267101	-0.174129	2.909466
31	1	0	3.512790	-1.289049	2.346742
32	1	0	-2.269100	-0.180445	-2.913455
33	1	0	-3.527283	-1.276865	-2.341545
34	6	0	3.145414	0.425217	1.084932
35	6	0	4.417549	0.999114	1.184578
36	6	0	4.734779	2.079266	0.359002
37	1	0	5.137640	0.608521	1.895706
38	6	0	2.544460	1.923333	-0.600111
39	6	0	3.783066	2.557414	-0.546299
40	1	0	5.715278	2.540692	0.420115
41	1	0	3.981003	3.393265	-1.206797
42	6	0	-3.139906	0.441513	-1.091189
43	6	0	-4.406750	1.027212	-1.189171
44	6	0	-2.523094	1.933862	0.594324
45	6	0	-4.712229	2.110991	-0.363732
46	1	0	-5.132330	0.642295	-1.897833
47	6	0	-3.755770	2.579635	0.541683
48	1	0	-5.688530	2.581414	-0.423596
49	1	0	-3.946601	3.415664	1.204051
50	7	0	-2.232597	0.889951	-0.208887
51	7	0	2.243515	0.879909	0.200156
52	6	0	1.445729	2.341022	-1.563536
53	8	0	0.373010	1.605243	-1.502972
54	8	0	1.630999	3.304665	-2.311839
55	6	0	-1.422866	2.332495	1.564730
56	8	0	-1.596563	3.298538	2.312674
57	8	0	-0.363879	1.576167	1.513062
58	7	0	-1.430165	-1.555533	1.604826
59	7	0	1.411534	-1.590110	-1.593690
60	6	0	-1.987349	-0.814921	2.766652
61	1	0	-1.183779	-0.355316	3.342339
62	1	0	-2.649947	-0.026170	2.408551
63	1	0	-2.558867	-1.493179	3.416285
64	6	0	1.972101	-0.857930	-2.759757
65	1	0	1.170428	-0.397600	-3.337844

66	1	0	2.638006	-0.070117	-2.405160
67	1	0	2.540246	-1.541421	-3.406703

E(RTPSSh) = -1602.90155617

Zero-point correction= 0.560902 (Hartree/Particle)

Thermal correction to Energy= 0.592125

Thermal correction to Enthalpy= 0.593069

Thermal correction to Gibbs Free Energy= 0.501300

Sum of electronic and zero-point Energies= -1602.340655

Sum of electronic and thermal Energies= -1602.309432

Sum of electronic and thermal Enthalpies= -1602.308487

Sum of electronic and thermal Free Energies= -1602.400256

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	70	0	0.000000	0.063393	0.000000
2	7	0	1.672787	1.172980	1.561010
3	6	0	0.895354	1.814608	2.660512
4	6	0	-0.245102	2.712940	2.177858
5	6	0	-1.888942	2.874092	0.349132
6	6	0	-2.554197	2.122136	-0.813390
7	7	0	-1.672787	1.172980	-1.561010
8	6	0	-0.895354	1.814608	-2.660511
9	6	0	0.245102	2.712940	-2.177858
10	6	0	1.888942	2.874092	-0.349132
11	6	0	2.554197	2.122136	0.813391
12	6	0	2.519894	0.087360	2.151804
13	6	0	-2.519894	0.087360	-2.151804
14	1	0	1.559219	2.403159	3.313162
15	1	0	0.477781	0.997922	3.255797
16	1	0	-1.140090	3.575527	-0.021161
17	1	0	-2.665938	3.478834	0.843744
18	1	0	-3.387024	1.533374	-0.418139

19	1	0	-2.988452	2.860755	-1.504374
20	1	0	-1.559219	2.403160	-3.313162
21	1	0	-0.477781	0.997923	-3.255796
22	1	0	1.140090	3.575527	0.021162
23	1	0	2.665938	3.478835	-0.843743
24	1	0	3.387025	1.533373	0.418139
25	1	0	2.988453	2.860754	1.504376
26	1	0	3.367169	0.509299	2.711070
27	1	0	1.885416	-0.468499	2.850059
28	1	0	-3.367169	0.509299	-2.711069
29	1	0	-1.885416	-0.468499	-2.850059
30	6	0	2.990876	-0.882530	1.087324
31	6	0	4.165681	-1.634294	1.159805
32	6	0	4.431316	-2.562182	0.145147
33	1	0	4.852311	-1.505966	1.990699
34	6	0	2.393641	-1.911734	-0.929138
35	6	0	3.537341	-2.708097	-0.918852
36	1	0	5.335904	-3.161484	0.185921
37	1	0	3.701590	-3.406079	-1.732049
38	6	0	-2.990876	-0.882529	-1.087324
39	6	0	-4.165682	-1.634293	-1.159805
40	6	0	-2.393641	-1.911735	0.929137
41	6	0	-4.431315	-2.562181	-0.145147
42	1	0	-4.852312	-1.505965	-1.990699
43	6	0	-3.537341	-2.708098	0.918852
44	1	0	-5.335905	-3.161483	-0.185921
45	1	0	-3.701589	-3.406080	1.732048
46	7	0	-2.142645	-1.029709	-0.056346
47	7	0	2.142645	-1.029708	0.056345
48	6	0	1.357463	-1.937142	-2.046637
49	8	0	0.343845	-1.126426	-1.830223
50	8	0	1.538752	-2.648652	-3.023443
51	6	0	-1.357463	-1.937143	2.046636
52	8	0	-1.538752	-2.648653	3.023443
53	8	0	-0.343845	-1.126427	1.830222
54	1	0	0.750200	3.129133	-3.061735

55	1	0	-0.140021	3.566453	-1.617600
56	1	0	0.140022	3.566453	1.617601
57	1	0	-0.750200	3.129133	3.061736
58	7	0	1.222864	1.971988	-1.325005
59	7	0	-1.222864	1.971988	1.325006
60	6	0	2.247248	1.364215	-2.217196
61	1	0	2.949761	0.771046	-1.631696
62	1	0	1.762058	0.703987	-2.936063
63	1	0	2.798809	2.151365	-2.752295
64	6	0	-2.247248	1.364214	2.217197
65	1	0	-2.949762	0.771046	1.631696
66	1	0	-1.762059	0.703986	2.936062
67	1	0	-2.798809	2.151366	2.752296

E(RTPSSh) = -1602.89912652

Zero-point correction= 0.561086 (Hartree/Particle)

Thermal correction to Energy= 0.592254

Thermal correction to Enthalpy= 0.593198

Thermal correction to Gibbs Free Energy= 0.502528

Sum of electronic and zero-point Energies= -1602.340008

Sum of electronic and thermal Energies= -1602.308840

Sum of electronic and thermal Enthalpies= -1602.307896

Sum of electronic and thermal Free Energies= -1602.398566

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.515524	-1.849009	1.001174
2	6	0	-0.747638	-2.733457	1.934019
3	6	0	0.291244	-1.986698	2.766154
4	6	0	2.390892	-1.961507	1.404899
5	6	0	2.083242	-2.693613	0.097950
6	7	0	1.515524	-1.849009	-1.001174
7	6	0	0.747637	-2.733457	-1.934019

8	6	0	-0.291244	-1.986698	-2.766154
9	6	0	-2.390892	-1.961507	-1.404899
10	6	0	-2.083242	-2.693613	-0.097950
11	6	0	-2.605982	-1.171980	1.777103
12	6	0	2.605982	-1.171981	-1.777103
13	1	0	-0.265318	-3.505925	1.334239
14	1	0	-1.431353	-3.257029	2.619657
15	1	0	3.208597	-1.257900	1.234774
16	1	0	2.759986	-2.710937	2.124837
17	1	0	3.012126	-3.176476	-0.242084
18	1	0	1.373098	-3.500763	0.283792
19	1	0	0.265317	-3.505925	-1.334238
20	1	0	1.431353	-3.257029	-2.619657
21	1	0	-3.208597	-1.257900	-1.234774
22	1	0	-2.759986	-2.710937	-2.124837
23	1	0	-3.012126	-3.176475	0.242084
24	1	0	-1.373099	-3.500763	-0.283792
25	1	0	-3.418821	-1.884600	1.980857
26	1	0	-2.184473	-0.885982	2.747912
27	1	0	3.418821	-1.884600	-1.980858
28	1	0	2.184472	-0.885982	-2.747912
29	6	0	-3.142302	0.083155	1.114976
30	6	0	-4.424765	0.587480	1.337278
31	6	0	-4.776845	1.802718	0.735955
32	1	0	-5.129382	0.052640	1.966690
33	6	0	-2.608578	1.884823	-0.282400
34	6	0	-3.862699	2.463231	-0.087534
35	1	0	-5.765440	2.219978	0.902604
36	1	0	-4.091107	3.396164	-0.590454
37	6	0	3.142302	0.083155	-1.114976
38	6	0	4.424765	0.587480	-1.337278
39	6	0	2.608579	1.884823	0.282400
40	6	0	4.776845	1.802718	-0.735955
41	1	0	5.129382	0.052640	-1.966690
42	6	0	3.862699	2.463230	0.087534
43	1	0	5.765440	2.219977	-0.902604

44	1	0	4.091107	3.396164	0.590454
45	7	0	2.269705	0.730881	-0.327016
46	7	0	-2.269705	0.730881	0.327016
47	6	0	-1.566536	2.458365	-1.243312
48	8	0	-0.496986	1.710600	-1.353412
49	8	0	-1.826494	3.491251	-1.843259
50	6	0	1.566536	2.458365	1.243312
51	8	0	1.826495	3.491251	1.843259
52	8	0	0.496986	1.710600	1.353412
53	1	0	-0.807972	-2.718202	-3.409086
54	1	0	0.217675	-1.289269	-3.439191
55	1	0	-0.217675	-1.289269	3.439191
56	1	0	0.807972	-2.718202	3.409086
57	7	0	-1.275701	-1.173676	-2.000137
58	7	0	1.275701	-1.173676	2.000137
59	6	0	-1.895821	-0.250476	-2.997078
60	1	0	-2.664256	0.349901	-2.510589
61	1	0	-1.138132	0.424370	-3.394113
62	1	0	-2.357536	-0.824340	-3.814576
63	6	0	1.895821	-0.250476	2.997078
64	1	0	2.664256	0.349900	2.510590
65	1	0	1.138132	0.424370	3.394113
66	1	0	2.357536	-0.824340	3.814576
67	70	0	0.000000	0.060113	0.000000

E(RTPSSh) = -1602.88035215

Zero-point correction= 0.562647 (Hartree/Particle)

Thermal correction to Energy= 0.593245

Thermal correction to Enthalpy= 0.594189

Thermal correction to Gibbs Free Energy= 0.504858

Sum of electronic and zero-point Energies= -1602.322315

Sum of electronic and thermal Energies= -1602.291717

Sum of electronic and thermal Enthalpies= -1602.290773

Sum of electronic and thermal Free Energies= -1602.380104

[Lu(Me$_2$dodpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.000000	0.066908
2	7	0	1.077551	1.836564	1.562812
3	6	0	1.993697	1.261898	2.585907
4	6	0	2.740294	0.029030	2.086641
5	6	0	1.143992	-1.731999	2.733249
6	6	0	0.000000	-2.620195	2.239642
7	7	0	-1.077551	-1.836564	1.562812
8	6	0	-1.993697	-1.261898	2.585907
9	6	0	-2.740294	-0.029030	2.086641
10	6	0	-1.143992	1.731999	2.733249
11	6	0	0.000000	2.620195	2.239642
12	6	0	1.831975	2.729504	0.629662
13	6	0	-1.831975	-2.729504	0.629662
14	1	0	1.393933	1.013462	3.466310
15	1	0	2.726412	2.014100	2.914539
16	1	0	3.375037	0.298302	1.236968
17	1	0	3.408159	-0.329971	2.886317
18	1	0	0.748951	-0.962293	3.404742
19	1	0	1.844095	-2.342385	3.326033
20	1	0	0.378913	-3.351831	1.523029
21	1	0	-0.417351	-3.184743	3.086398
22	1	0	-1.393933	-1.013462	3.466310
23	1	0	-2.726412	-2.014100	2.914539
24	1	0	-3.375037	-0.298302	1.236968
25	1	0	-3.408159	0.329971	2.886317
26	1	0	-0.748951	0.962293	3.404742
27	1	0	-1.844095	2.342385	3.326033
28	1	0	-0.378913	3.351831	1.523029
29	1	0	0.417351	3.184743	3.086398

30	1	0	2.185225	3.628720	1.156026
31	1	0	2.714397	2.181427	0.280007
32	1	0	-2.185225	-3.628720	1.156026
33	1	0	-2.714397	-2.181427	0.280007
34	6	0	0.982664	3.100433	-0.571922
35	6	0	1.136514	4.269761	-1.318256
36	6	0	0.316284	4.459415	-2.437835
37	1	0	1.878371	5.011545	-1.039247
38	6	0	-0.738748	2.360287	-1.973408
39	6	0	-0.640520	3.498096	-2.773174
40	1	0	0.421945	5.358646	-3.037193
41	1	0	-1.306265	3.604641	-3.622145
42	6	0	-0.982664	-3.100433	-0.571922
43	6	0	-1.136514	-4.269761	-1.318256
44	6	0	0.738748	-2.360287	-1.973408
45	6	0	-0.316284	-4.459415	-2.437835
46	1	0	-1.878371	-5.011545	-1.039247
47	6	0	0.640520	-3.498096	-2.773174
48	1	0	-0.421945	-5.358646	-3.037193
49	1	0	1.306265	-3.604641	-3.622145
50	7	0	-0.061325	-2.184075	-0.906004
51	7	0	0.061325	2.184075	-0.906004
52	6	0	-1.760424	1.251932	-2.202604
53	8	0	-1.623439	0.242331	-1.370626
54	8	0	-2.604557	1.383812	-3.076096
55	6	0	1.760424	-1.251932	-2.202604
56	8	0	2.604557	-1.383812	-3.076096
57	8	0	1.623439	-0.242331	-1.370626
58	7	0	1.850210	-1.065278	1.611261
59	7	0	-1.850210	1.065278	1.611261
60	6	0	-2.722956	2.051871	0.920685
61	1	0	-2.126091	2.869552	0.517913
62	1	0	-3.230504	1.558772	0.091608
63	1	0	-3.467727	2.462403	1.619242
64	6	0	2.722956	-2.051871	0.920685
65	1	0	2.126091	-2.869552	0.517913

66	1	0	3.230504	-1.558772	0.091608
67	1	0	3.467727	-2.462403	1.619242

E(RTPSSh) = -1603.45431865

Zero-point correction= 0.561074 (Hartree/Particle)

Thermal correction to Energy= 0.592166

Thermal correction to Enthalpy= 0.593110

Thermal correction to Gibbs Free Energy= 0.503367

Sum of electronic and zero-point Energies= -1602.896726

Sum of electronic and thermal Energies= -1602.865634

Sum of electronic and thermal Enthalpies= -1602.864690

Sum of electronic and thermal Free Energies= -1602.954432

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.000000	0.052379
2	7	0	1.318665	-1.687138	1.490380
3	6	0	0.424809	-2.234173	2.560772
4	6	0	-1.007716	-2.502866	2.113120
5	6	0	-2.106969	-0.384139	2.663763
6	6	0	-2.478117	1.004210	2.150500
7	7	0	-1.318665	1.687138	1.490380
8	6	0	-0.424809	2.234173	2.560772
9	6	0	1.007716	2.502866	2.113120
10	6	0	2.106969	0.384139	2.663763
11	6	0	2.478117	-1.004210	2.150500
12	6	0	1.829929	-2.787752	0.618934
13	6	0	-1.829929	2.787752	0.618934
14	1	0	0.425897	-1.518446	3.385906
15	1	0	0.852245	-3.165959	2.955660
16	1	0	-1.024767	-3.271658	1.338043
17	1	0	-1.569086	-2.900100	2.971892
18	1	0	-1.287311	-0.317788	3.383719

19	1	0	-2.967226	-0.807571	3.202178
20	1	0	-3.281839	0.926954	1.415477
21	1	0	-2.856816	1.611363	2.983645
22	1	0	-0.425897	1.518446	3.385906
23	1	0	-0.852245	3.165959	2.955660
24	1	0	1.024767	3.271658	1.338043
25	1	0	1.569086	2.900100	2.971892
26	1	0	1.287311	0.317788	3.383719
27	1	0	2.967226	0.807571	3.202178
28	1	0	3.281839	-0.926954	1.415477
29	1	0	2.856816	-1.611363	2.983645
30	1	0	2.737312	-2.420479	0.126959
31	1	0	2.117727	-3.659925	1.220238
32	1	0	-2.737312	2.420479	0.126959
33	1	0	-2.117727	3.659925	1.220238
34	6	0	0.859092	-3.184581	-0.471720
35	6	0	0.865170	-4.446834	-1.075356
36	6	0	0.000000	-4.683516	-2.145766
37	1	0	1.533649	-5.221623	-0.715575
38	6	0	-0.812900	-2.441424	-1.921786
39	6	0	-0.852213	-3.665720	-2.583993
40	1	0	-0.011138	-5.654815	-2.629963
41	1	0	-1.541052	-3.802566	-3.409213
42	6	0	-0.859092	3.184581	-0.471720
43	6	0	-0.865170	4.446834	-1.075356
44	6	0	0.812900	2.441424	-1.921786
45	6	0	0.000000	4.683516	-2.145766
46	1	0	-1.533649	5.221623	-0.715575
47	6	0	0.852213	3.665720	-2.583993
48	1	0	0.011138	5.654815	-2.629963
49	1	0	1.541052	3.802566	-3.409213
50	7	0	-0.027106	2.218677	-0.891358
51	7	0	0.027106	-2.218677	-0.891358
52	6	0	-1.711907	-1.271429	-2.285754
53	8	0	-1.563083	-0.225814	-1.522246
54	8	0	-2.495361	-1.380694	-3.232491

55	6	0	1.711907	1.271429	-2.285754
56	8	0	2.495361	1.380694	-3.232491
57	8	0	1.563083	0.225814	-1.522246
58	7	0	1.692073	1.297834	1.559547
59	7	0	-1.692073	-1.297834	1.559547
60	6	0	2.912600	1.764105	0.849773
61	1	0	3.435003	0.921948	0.396214
62	1	0	2.627724	2.459606	0.059597
63	1	0	3.588152	2.277462	1.548752
64	6	0	-2.912600	-1.764105	0.849773
65	1	0	-3.435003	-0.921948	0.396214
66	1	0	-2.627724	-2.459606	0.059597
67	1	0	-3.588152	-2.277462	1.548752

E(RTPSSh) = -1603.45602079

Zero-point correction= 0.562096 (Hartree/Particle)

Thermal correction to Energy= 0.592820

Thermal correction to Enthalpy= 0.593764

Thermal correction to Gibbs Free Energy= 0.504952

Sum of electronic and zero-point Energies= -1602.894365

Sum of electronic and thermal Energies= -1602.863641

Sum of electronic and thermal Enthalpies= -1602.862697

Sum of electronic and thermal Free Energies= -1602.951510

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.070189	0.000000
2	7	0	-1.671124	1.170216	-1.556721
3	6	0	-0.897627	1.812191	-2.658653
4	6	0	0.243042	2.710274	-2.177410
5	6	0	1.888539	2.871094	-0.351281
6	6	0	2.554132	2.118731	0.810163
7	7	0	1.671124	1.170216	1.556721

8	6	0	0.897628	1.812192	2.658653
9	6	0	-0.243041	2.710275	2.177409
10	6	0	-1.888538	2.871094	0.351280
11	6	0	-2.554132	2.118731	-0.810164
12	6	0	-2.517652	0.083051	-2.145240
13	6	0	2.517652	0.083052	2.145240
14	1	0	-1.563624	2.400432	-3.309329
15	1	0	-0.481043	0.995778	-3.254799
16	1	0	1.140660	3.573238	0.019679
17	1	0	2.664888	3.474813	-0.848026
18	1	0	3.386156	1.529291	0.414205
19	1	0	2.989395	2.856237	1.501622
20	1	0	1.563625	2.400432	3.309329
21	1	0	0.481043	0.995778	3.254798
22	1	0	-1.140659	3.573238	-0.019680
23	1	0	-2.664887	3.474814	0.848025
24	1	0	-3.386155	1.529292	-0.414206
25	1	0	-2.989394	2.856237	-1.501622
26	1	0	-3.368398	0.503375	-2.700379
27	1	0	-1.884577	-0.471063	-2.845958
28	1	0	3.368398	0.503375	2.700378
29	1	0	1.884577	-0.471063	2.845958
30	6	0	-2.980470	-0.888100	-1.078959
31	6	0	-4.150460	-1.647688	-1.148083
32	6	0	-4.407659	-2.576701	-0.132441
33	1	0	-4.839759	-1.524463	-1.977540
34	6	0	-2.371700	-1.912248	0.935958
35	6	0	-3.509901	-2.716310	0.929237
36	1	0	-5.308370	-3.181980	-0.170704
37	1	0	-3.667135	-3.415194	1.743047
38	6	0	2.980470	-0.888099	1.078960
39	6	0	4.150460	-1.647688	1.148084
40	6	0	2.371700	-1.912249	-0.935958
41	6	0	4.407658	-2.576702	0.132442
42	1	0	4.839758	-1.524464	1.977540
43	6	0	3.509901	-2.716312	-0.929236

44	1	0	5.308369	-3.181981	0.170704
45	1	0	3.667134	-3.415195	-1.743047
46	7	0	2.128774	-1.028509	0.049999
47	7	0	-2.128775	-1.028509	-0.049998
48	6	0	-1.331023	-1.929371	2.048546
49	8	0	-0.324761	-1.111294	1.825373
50	8	0	-1.501346	-2.640610	3.027477
51	6	0	1.331023	-1.929372	-2.048545
52	8	0	1.501346	-2.640610	-3.027476
53	8	0	0.324760	-1.111294	-1.825372
54	1	0	-0.748478	3.126253	3.061138
55	1	0	0.141266	3.563879	1.616714
56	1	0	-0.141265	3.563879	-1.616715
57	1	0	0.748479	3.126252	-3.061138
58	7	0	-1.220213	1.967970	1.324806
59	7	0	1.220213	1.967969	-1.324806
60	6	0	-2.243439	1.360115	2.218531
61	1	0	-2.946584	0.766546	1.634347
62	1	0	-1.757138	0.700870	2.937433
63	1	0	-2.794469	2.147561	2.753660
64	6	0	2.243440	1.360113	-2.218530
65	1	0	2.946583	0.766544	-1.634347
66	1	0	1.757138	0.700868	-2.937434
67	1	0	2.794470	2.147559	-2.753660

E(RTPSSh) = -1603.45407611

Zero-point correction= 0.561801 (Hartree/Particle)

Thermal correction to Energy= 0.592748

Thermal correction to Enthalpy= 0.593692

Thermal correction to Gibbs Free Energy= 0.504394

Sum of electronic and zero-point Energies= -1602.894351

Sum of electronic and thermal Energies= -1602.863404

Sum of electronic and thermal Enthalpies= -1602.862459

Sum of electronic and thermal Free Energies= -1602.951758

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	71	0	0.000000	0.050186	0.000000
2	7	0	-1.513533	-1.848107	0.998915
3	6	0	-0.749359	-2.731996	1.935423
4	6	0	0.289121	-1.984112	2.766489
5	6	0	2.388607	-1.963679	1.405635
6	6	0	2.080290	-2.695015	0.098826
7	7	0	1.513533	-1.848107	-0.998915
8	6	0	0.749359	-2.731996	-1.935423
9	6	0	-0.289121	-1.984112	-2.766489
10	6	0	-2.388607	-1.963679	-1.405635
11	6	0	-2.080290	-2.695015	-0.098826
12	6	0	-2.604876	-1.167683	1.770934
13	6	0	2.604876	-1.167683	-1.770934
14	1	0	-0.267356	-3.506894	1.338492
15	1	0	-1.435396	-3.252432	2.621046
16	1	0	3.208025	-1.261836	1.236216
17	1	0	2.755180	-2.713297	2.126587
18	1	0	3.008133	-3.179216	-0.242076
19	1	0	1.368578	-3.500896	0.284165
20	1	0	0.267356	-3.506894	-1.338492
21	1	0	1.435396	-3.252432	-2.621046
22	1	0	-3.208025	-1.261836	-1.236216
23	1	0	-2.755180	-2.713297	-2.126587
24	1	0	-3.008133	-3.179216	0.242076
25	1	0	-1.368578	-3.500896	-0.284165
26	1	0	-3.421879	-1.876969	1.969276
27	1	0	-2.186852	-0.885179	2.744212
28	1	0	3.421880	-1.876969	-1.969276
29	1	0	2.186852	-0.885179	-2.744212
30	6	0	-3.131325	0.091286	1.108309
31	6	0	-4.408390	0.608678	1.332322

32	6	0	-4.748811	1.827207	0.731115
33	1	0	-5.117429	0.081439	1.963175
34	6	0	-2.581167	1.887562	-0.289574
35	6	0	-3.828937	2.478698	-0.093350
36	1	0	-5.732878	2.254549	0.899020
37	1	0	-4.048478	3.414233	-0.595389
38	6	0	3.131325	0.091286	-1.108309
39	6	0	4.408390	0.608678	-1.332322
40	6	0	2.581167	1.887562	0.289574
41	6	0	4.748811	1.827207	-0.731116
42	1	0	5.117429	0.081439	-1.963175
43	6	0	3.828937	2.478698	0.093350
44	1	0	5.732878	2.254549	-0.899021
45	1	0	4.048478	3.414233	0.595388
46	7	0	2.253831	0.729774	-0.318747
47	7	0	-2.253831	0.729774	0.318747
48	6	0	-1.532318	2.450134	-1.248938
49	8	0	-0.469895	1.691451	-1.356682
50	8	0	-1.779906	3.485475	-1.849733
51	6	0	1.532318	2.450134	1.248938
52	8	0	1.779905	3.485475	1.849733
53	8	0	0.469895	1.691451	1.356683
54	1	0	-0.805594	-2.713999	-3.411405
55	1	0	0.219793	-1.284619	-3.437333
56	1	0	-0.219793	-1.284619	3.437333
57	1	0	0.805594	-2.713999	3.411405
58	7	0	-1.273621	-1.173505	-1.997936
59	7	0	1.273621	-1.173505	1.997936
60	6	0	-1.894175	-0.248585	-2.993007
61	1	0	-2.661633	0.351863	-2.504993
62	1	0	-1.136143	0.425521	-3.390396
63	1	0	-2.357570	-0.821368	-3.810308
64	6	0	1.894175	-0.248585	2.993007
65	1	0	2.661633	0.351863	2.504993
66	1	0	1.136143	0.425521	3.390396
67	1	0	2.357570	-0.821368	3.810308

E(RTPSSh) = -1603.43387575

Zero-point correction= 0.562669 (Hartree/Particle)

Thermal correction to Energy= 0.593310

Thermal correction to Enthalpy= 0.594254

Thermal correction to Gibbs Free Energy= 0.504792

Sum of electronic and zero-point Energies= -1602.875011

Sum of electronic and thermal Energies= -1602.844370

Sum of electronic and thermal Enthalpies= -1602.843425

Sum of electronic and thermal Free Energies= -1602.932888

Complejos de H_2Me_2TEDPA

Las geometrías optimizadas en disolución se corresponden con las siguientes conformaciones:

- F1: Λ(δδ)
- F2: Δ(λδ)
- F3: Λ(δλ)
- F4: Λ(λλ)

[La(Me_2tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.890715	2.475343	-1.712517
2	6	0	-2.893169	2.060638	-0.643558
3	6	0	-4.184903	2.584457	-0.605257
4	1	0	-4.479122	3.316786	-1.347745
5	6	0	-5.057682	2.133072	0.387054
6	1	0	-6.074150	2.510210	0.439837
7	6	0	-4.613541	1.183400	1.309384
8	1	0	-5.271507	0.809760	2.086866
9	6	0	-3.297903	0.715218	1.217099
10	6	0	-2.715932	-0.230610	2.244628
11	1	0	-2.215277	0.386780	3.000271
12	1	0	-3.522249	-0.772390	2.758486
13	6	0	-2.358632	-2.353566	1.067761
14	1	0	-3.204613	-2.705318	1.677536
15	1	0	-1.640488	-3.174038	1.027762
16	6	0	-2.877208	-2.051901	-0.337819
17	1	0	-3.427089	-2.941020	-0.687391
18	1	0	-3.595860	-1.230346	-0.307893
19	6	0	1.069585	-2.921157	1.691140
20	1	0	1.782767	-3.713481	1.973672
21	1	0	0.564812	-3.270179	0.787568
22	6	0	-0.933127	-1.636772	2.951271
23	1	0	-1.651202	-1.910477	3.739296

24	1	0	-0.403989	-0.747310	3.308087
25	6	0	-2.509832	-1.154789	-2.527442
26	1	0	-3.168507	-1.911413	-2.981853
27	1	0	-1.778996	-0.831407	-3.269964
28	1	0	-3.113729	-0.291663	-2.239793
29	6	0	0.048765	-2.815745	2.837939
30	1	0	0.583550	-2.815971	3.795241
31	1	0	-0.508875	-3.759422	2.823134
32	7	0	-2.466242	1.149166	0.253622
33	7	0	-1.697308	-1.197225	1.733318
34	7	0	-1.823635	-1.690827	-1.328067
35	8	0	-0.749800	1.859381	-1.659444
36	8	0	-2.223989	3.336317	-2.535330
37	6	0	1.890643	2.475380	1.712500
38	6	0	2.893124	2.060682	0.643561
39	6	0	4.184850	2.584520	0.605272
40	1	0	4.479051	3.316857	1.347757
41	6	0	5.057645	2.133145	-0.387030
42	1	0	6.074108	2.510300	-0.439804
43	6	0	4.613527	1.183465	-1.309363
44	1	0	5.271506	0.809837	-2.086841
45	6	0	3.297896	0.715263	-1.217091
46	6	0	2.715947	-0.230575	-2.244626
47	1	0	2.215285	0.386812	-3.000268
48	1	0	3.522278	-0.772335	-2.758485
49	6	0	2.358672	-2.353542	-1.067760
50	1	0	3.204661	-2.705285	-1.677531
51	1	0	1.640539	-3.174024	-1.027770
52	6	0	2.877244	-2.051880	0.337824
53	1	0	3.427128	-2.940997	0.687397
54	1	0	3.595896	-1.230324	0.307901
55	6	0	-1.069502	-2.921172	-1.691062
56	1	0	-1.782657	-3.713540	-1.973536
57	1	0	-0.564706	-3.270110	-0.787471
58	6	0	0.933163	-1.636796	-2.951264
59	1	0	1.651244	-1.910518	-3.739279

60	1	0	0.404008	-0.747358	-3.308111
61	6	0	2.509915	-1.154709	2.527404
62	1	0	3.168618	-1.911308	2.981818
63	1	0	1.779107	-0.831308	3.269945
64	1	0	3.113792	-0.291588	2.239698
65	6	0	-0.048704	-2.815786	-2.837881
66	1	0	-0.583501	-2.816060	-3.795176
67	1	0	0.508955	-3.759451	-2.823038
68	7	0	2.466221	1.149200	-0.253619
69	7	0	1.697340	-1.197211	-1.733322
70	7	0	1.823679	-1.690804	1.328075
71	8	0	0.749731	1.859417	1.659393
72	8	0	2.223897	3.336347	2.535330
73	57	0	-0.000012	0.201053	-0.000017

E(RTPSSh) = -1673.69345808

Zero-point correction= 0.618835 (Hartree/Particle)

Thermal correction to Energy= 0.652339

Thermal correction to Enthalpy= 0.653283

Thermal correction to Gibbs Free Energy= 0.557354

Sum of electronic and zero-point Energies= -1673.074623

Sum of electronic and thermal Energies= -1673.041119

Sum of electronic and thermal Enthalpies= -1673.040175

Sum of electronic and thermal Free Energies= -1673.136104

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.320981	-2.694610	1.574696
2	6	0	-2.482867	-2.352239	0.653586
3	6	0	-3.684341	-3.058291	0.689640
4	1	0	-3.791039	-3.883806	1.383438
5	6	0	-4.712841	-2.665028	-0.169168
6	1	0	-5.665195	-3.185777	-0.162716

7	6	0	-4.508935	-1.588219	-1.034458
8	1	0	-5.292529	-1.257163	-1.707739
9	6	0	-3.269810	-0.937118	-1.024367
10	6	0	-2.940556	0.163303	-2.009283
11	1	0	-2.459687	-0.314276	-2.872211
12	1	0	-3.866145	0.628048	-2.378113
13	6	0	-2.709637	2.193490	-0.651585
14	1	0	-3.685108	2.453259	-1.090541
15	1	0	-2.124227	3.112025	-0.630218
16	6	0	-2.962963	1.701968	0.776757
17	1	0	-3.553763	2.478176	1.290247
18	1	0	-3.579507	0.801184	0.757107
19	6	0	0.284925	3.544508	-1.532005
20	1	0	0.839692	4.443088	-1.852529
21	1	0	-0.296669	3.851849	-0.660367
22	6	0	-1.434511	1.847108	-2.763818
23	1	0	-2.254290	2.012555	-3.478868
24	1	0	-0.786922	1.086570	-3.212909
25	6	0	-2.218715	0.688604	2.806688
26	1	0	-2.899967	1.327341	3.390197
27	1	0	-1.373292	0.408240	3.435342
28	1	0	-2.750829	-0.220344	2.518871
29	6	0	-0.676515	3.188808	-2.679370
30	1	0	-0.144438	3.258243	-3.635620
31	1	0	-1.402745	4.010178	-2.695266
32	7	0	-2.286789	-1.319450	-0.190848
33	7	0	-1.999513	1.214007	-1.519098
34	7	0	-1.747756	1.386259	1.586869
35	8	0	-0.282318	-1.927124	1.445302
36	8	0	-1.439923	-3.643339	2.358457
37	6	0	1.827553	-2.336186	-2.045698
38	6	0	2.892342	-1.998057	-1.011628
39	6	0	4.191862	-2.500360	-1.091641
40	1	0	4.459552	-3.146352	-1.919405
41	6	0	5.105451	-2.144252	-0.097905
42	1	0	6.127675	-2.507746	-0.133851

43	6	0	4.693873	-1.313003	0.947500
44	1	0	5.381283	-1.023067	1.735145
45	6	0	3.371361	-0.859305	0.964502
46	6	0	2.798297	-0.046921	2.101800
47	1	0	2.232341	-0.728216	2.747361
48	1	0	3.606170	0.383494	2.710289
49	6	0	2.690115	2.092764	1.005972
50	1	0	3.447141	1.575565	0.408834
51	1	0	3.230139	2.660063	1.779294
52	6	0	1.947206	3.093482	0.122515
53	1	0	1.206146	3.628806	0.717256
54	1	0	2.682654	3.845979	-0.206392
55	6	0	-1.080223	2.661308	1.964140
56	1	0	-1.821019	3.334220	2.427359
57	1	0	-0.775142	3.141512	1.033270
58	6	0	1.166387	1.466654	2.913311
59	1	0	1.935649	1.755620	3.646611
60	1	0	0.695602	0.558128	3.299767
61	6	0	2.216980	2.210968	-2.134125
62	1	0	2.752508	3.117973	-2.456469
63	1	0	1.690490	1.785314	-2.991647
64	1	0	2.944176	1.475230	-1.783071
65	6	0	0.125899	2.601695	2.926877
66	1	0	-0.254167	2.576196	3.955461
67	1	0	0.629054	3.571252	2.835747
68	7	0	2.503351	-1.193496	-0.005669
69	7	0	1.858639	1.031293	1.654464
70	7	0	1.246189	2.517240	-1.059510
71	8	0	0.664029	-1.805274	-1.822505
72	8	0	2.130459	-3.071798	-2.992986
73	57	0	0.060762	-0.116675	-0.150717

E(RTPSSh) = -1673.68729032

Zero-point correction= 0.618637 (Hartree/Particle)

Thermal correction to Energy= 0.652313

Thermal correction to Enthalpy= 0.653257

Thermal correction to Gibbs Free Energy= 0.557226

Sum of electronic and zero-point Energies= -1673.068654

Sum of electronic and thermal Energies= -1673.034977

Sum of electronic and thermal Enthalpies= -1673.034033

Sum of electronic and thermal Free Energies= -1673.130064

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.029689	-2.205013	-2.084929
2	6	0	3.046023	-1.810502	-1.022851
3	6	0	4.368920	-2.252456	-1.056382
4	1	0	4.692800	-2.894136	-1.867368
5	6	0	5.232386	-1.843006	-0.038029
6	1	0	6.271456	-2.157310	-0.037943
7	6	0	4.747764	-1.025914	0.986709
8	1	0	5.394484	-0.699418	1.794299
9	6	0	3.403398	-0.640421	0.960595
10	6	0	2.749508	0.115178	2.093158
11	1	0	2.240177	-0.623849	2.721341
12	1	0	3.507821	0.609441	2.716174
13	6	0	2.444355	2.290788	1.100777
14	1	0	3.270551	1.894453	0.502294
15	1	0	2.895778	2.869896	1.920274
16	6	0	1.612431	3.249377	0.248576
17	1	0	0.820354	3.691051	0.853779
18	1	0	2.272811	4.078179	-0.052650
19	6	0	-1.364449	2.467477	1.984486
20	1	0	-2.152422	3.088425	2.443362
21	1	0	-1.073826	2.971754	1.061705
22	6	0	0.931210	1.386032	2.907916
23	1	0	1.643349	1.651229	3.704946
24	1	0	0.499568	0.417638	3.176980
25	6	0	1.980760	2.491509	-2.037142

26	1	0	2.403771	3.466399	-2.323469
27	1	0	1.514425	2.034660	-2.913222
28	1	0	2.791601	1.839032	-1.704922
29	6	0	-0.172218	2.456142	2.962430
30	1	0	-0.562509	2.359926	3.983030
31	1	0	0.269947	3.458505	2.923846
32	7	0	2.586366	-1.020513	-0.035682
33	7	0	1.716406	1.109503	1.657533
34	7	0	0.975460	2.646535	-0.959349
35	8	0	0.840949	-1.711428	-1.910732
36	8	0	2.388789	-2.947058	-3.007100
37	6	0	-1.003711	-2.628513	1.633107
38	6	0	-2.179344	-2.477179	0.675147
39	6	0	-3.295346	-3.311575	0.731460
40	1	0	-3.319825	-4.113572	1.459715
41	6	0	-4.352094	-3.069229	-0.149265
42	1	0	-5.239895	-3.693390	-0.127714
43	6	0	-4.267207	-2.004621	-1.049747
44	1	0	-5.082096	-1.783856	-1.731059
45	6	0	-3.110278	-1.217532	-1.056485
46	6	0	-2.904715	-0.089738	-2.046976
47	1	0	-2.356883	-0.500974	-2.904040
48	1	0	-3.874776	0.261744	-2.426087
49	6	0	-2.934170	1.930834	-0.652635
50	1	0	-3.925626	2.089929	-1.103953
51	1	0	-2.458017	2.909421	-0.601544
52	6	0	-3.155797	1.383402	0.760723
53	1	0	-3.821026	2.093282	1.280391
54	1	0	-3.692423	0.434061	0.710343
55	6	0	-0.076845	3.594746	-1.414559
56	1	0	0.396893	4.551429	-1.691424
57	1	0	-0.700349	3.814479	-0.545986
58	6	0	-1.596851	1.783646	-2.743649
59	1	0	-2.417749	1.891471	-3.468492
60	1	0	-0.868079	1.111028	-3.208714
61	6	0	-2.366889	0.411194	2.786570

62	1	0	-3.104846	0.991192	3.363523
63	1	0	-1.514877	0.188345	3.428527
64	1	0	-2.825121	-0.532102	2.483538
65	6	0	-0.975321	3.189823	-2.597238
66	1	0	-0.431964	3.346226	-3.536505
67	1	0	-1.777433	3.937476	-2.602292
68	7	0	-2.095260	-1.466001	-0.211010
69	7	0	-2.105228	1.060909	-1.530316
70	7	0	-1.931536	1.154094	1.582971
71	8	0	-0.071609	-1.734621	1.503177
72	8	0	-1.022643	-3.555666	2.451592
73	57	0	0.113322	-0.050882	-0.259576

E(RTPSSh) = -1673.68749898

Zero-point correction= 0.618739 (Hartree/Particle)

Thermal correction to Energy= 0.652367

Thermal correction to Enthalpy= 0.653312

Thermal correction to Gibbs Free Energy= 0.557480

Sum of electronic and zero-point Energies= -1673.068760

Sum of electronic and thermal Energies= -1673.035132

Sum of electronic and thermal Enthalpies= -1673.034187

Sum of electronic and thermal Free Energies= -1673.130019

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.414992	2.315010	2.071835
2	6	0	2.513117	2.190784	1.021433
3	6	0	3.690123	2.937081	1.076940
4	1	0	3.844065	3.625569	1.899479
5	6	0	4.634551	2.764689	0.062149
6	1	0	5.564299	3.324689	0.077322
7	6	0	4.379245	1.863054	-0.975301
8	1	0	5.097967	1.711370	-1.773616

9	6	0	3.172743	1.156658	-0.967889
10	6	0	2.743335	0.227539	-2.083224
11	1	0	2.092001	0.792916	-2.759245
12	1	0	3.612718	-0.109392	-2.664556
13	6	0	2.913471	-1.850053	-0.870233
14	1	0	3.487412	-2.444755	-1.595664
15	1	0	3.628868	-1.197381	-0.361599
16	6	0	2.302081	-2.812442	0.150501
17	1	0	1.653885	-3.521139	-0.364465
18	1	0	3.127734	-3.402863	0.577541
19	6	0	-0.608432	-3.230834	-1.803491
20	1	0	-1.217051	-4.010082	-2.290069
21	1	0	-0.145196	-3.711821	-0.941961
22	6	0	1.284412	-1.513547	-2.810798
23	1	0	2.046035	-1.633008	-3.596255
24	1	0	0.614778	-0.714675	-3.149973
25	6	0	2.415114	-1.680517	2.309333
26	1	0	3.008188	-2.503664	2.735994
27	1	0	1.829951	-1.212896	3.104618
28	1	0	3.092771	-0.930212	1.896101
29	6	0	0.505113	-2.847199	-2.807469
30	1	0	0.086514	-2.875834	-3.820770
31	1	0	1.216928	-3.680836	-2.770517
32	7	0	2.276960	1.323788	0.019755
33	7	0	1.959824	-0.949457	-1.587900
34	7	0	1.506925	-2.177528	1.249556
35	8	0	0.352860	1.599521	1.846831
36	8	0	1.597862	3.071284	3.032530
37	6	0	-1.415119	2.314413	-2.072229
38	6	0	-2.513283	2.190393	-1.021847
39	6	0	-3.690140	2.936917	-1.077389
40	1	0	-3.843982	3.625342	-1.900000
41	6	0	-4.634536	2.764874	-0.062505
42	1	0	-5.564150	3.325093	-0.077673
43	6	0	-4.379350	1.863335	0.975050
44	1	0	-5.098036	1.711942	1.773453

45	6	0	-3.173028	1.156626	0.967612
46	6	0	-2.743718	0.227605	2.083074
47	1	0	-2.092631	0.793110	2.759229
48	1	0	-3.613159	-0.109481	2.664224
49	6	0	-2.913363	-1.850170	0.870323
50	1	0	-3.628617	-1.197592	0.361381
51	1	0	-3.487476	-2.444643	1.595820
52	6	0	-2.301747	-2.812808	-0.150002
53	1	0	-1.653416	-3.521173	0.365244
54	1	0	-3.127266	-3.403559	-0.576853
55	6	0	0.608816	-3.230250	1.804110
56	1	0	1.217562	-4.009248	2.290922
57	1	0	0.145678	-3.711555	0.942706
58	6	0	-1.284435	-1.513063	2.810968
59	1	0	-2.046064	-1.632559	3.596413
60	1	0	-0.614973	-0.714009	3.150051
61	6	0	-2.414968	-1.681462	-2.309108
62	1	0	-3.008111	-2.504742	-2.735430
63	1	0	-1.829853	-1.214156	-3.104613
64	1	0	-3.092557	-0.930973	-1.896100
65	6	0	-0.504835	-2.846549	2.807959
66	1	0	-0.086240	-2.874818	3.821273
67	1	0	-1.216463	-3.680356	2.771214
68	7	0	-2.277269	1.323423	-0.020104
69	7	0	-1.959905	-0.949290	1.587952
70	7	0	-1.506704	-2.178110	-1.249242
71	8	0	-0.352894	1.599162	-1.846843
72	8	0	-1.597986	3.070327	-3.033196
73	57	0	-0.000011	0.022364	0.000050

E(RTPSSh) = -1673.67637326

Zero-point correction= 0.618477 (Hartree/Particle)

Thermal correction to Energy= 0.652195

Thermal correction to Enthalpy= 0.653139

Thermal correction to Gibbs Free Energy= 0.557575

Sum of electronic and zero-point Energies= -1673.057896

Sum of electronic and thermal Energies= -1673.024179

Sum of electronic and thermal Enthalpies= -1673.023235

Sum of electronic and thermal Free Energies= -1673.118798

[Nd(Me$_2$tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.659416	2.281555	-1.823824
2	6	0	-2.667903	2.042276	-0.708310
3	6	0	-3.900637	2.690709	-0.660740
4	1	0	-4.153425	3.409436	-1.431272
5	6	0	-4.775884	2.375793	0.382591
6	1	0	-5.748637	2.853247	0.445458
7	6	0	-4.396433	1.434532	1.342218
8	1	0	-5.061589	1.168847	2.156935
9	6	0	-3.135707	0.836105	1.236451
10	6	0	-2.597457	-0.115497	2.283093
11	1	0	-2.067555	0.491991	3.026295
12	1	0	-3.422327	-0.616960	2.807385
13	6	0	-2.320522	-2.288516	1.156645
14	1	0	-3.152700	-2.616161	1.796869
15	1	0	-1.613888	-3.119076	1.109750
16	6	0	-2.875814	-2.004407	-0.239830
17	1	0	-3.434812	-2.896271	-0.564081
18	1	0	-3.592754	-1.181785	-0.198786
19	6	0	1.123064	-2.884857	1.679357
20	1	0	1.852853	-3.660804	1.961708
21	1	0	0.600692	-3.265793	0.797753
22	6	0	-0.809958	-1.539945	2.975155
23	1	0	-1.492671	-1.763795	3.807909
24	1	0	-0.243260	-0.647204	3.260204

25	6	0	-2.583332	-1.104523	-2.439649
26	1	0	-3.262737	-1.858199	-2.866059
27	1	0	-1.883178	-0.782141	-3.210511
28	1	0	-3.170920	-0.240569	-2.124731
29	6	0	0.135987	-2.747221	2.853903
30	1	0	0.700150	-2.743636	3.793907
31	1	0	-0.443475	-3.677257	2.871981
32	7	0	-2.304663	1.142546	0.227254
33	7	0	-1.619683	-1.128528	1.777982
34	7	0	-1.851803	-1.651017	-1.270262
35	8	0	-0.582904	1.552489	-1.750103
36	8	0	-1.920525	3.112573	-2.698777
37	6	0	1.659388	2.281594	1.823792
38	6	0	2.667891	2.042292	0.708297
39	6	0	3.900624	2.690727	0.660728
40	1	0	4.153406	3.409465	1.431251
41	6	0	4.775877	2.375801	-0.382596
42	1	0	5.748629	2.853258	-0.445463
43	6	0	4.396432	1.434533	-1.342218
44	1	0	5.061592	1.168843	-2.156929
45	6	0	3.135707	0.836104	-1.236453
46	6	0	2.597460	-0.115505	-2.283090
47	1	0	2.067562	0.491980	-3.026299
48	1	0	3.422332	-0.616970	-2.807376
49	6	0	2.320520	-2.288520	-1.156635
50	1	0	3.152698	-2.616169	-1.796858
51	1	0	1.613884	-3.119078	-1.109737
52	6	0	2.875816	-2.004405	0.239837
53	1	0	3.434812	-2.896270	0.564092
54	1	0	3.592759	-1.181786	0.198789
55	6	0	-1.123051	-2.884870	-1.679329
56	1	0	-1.852836	-3.660825	-1.961669
57	1	0	-0.600677	-3.265790	-0.797718
58	6	0	0.809961	-1.539963	-2.975148
59	1	0	1.492675	-1.763820	-3.807899
60	1	0	0.243257	-0.647230	-3.260206

61	6	0	2.583356	-1.104495	2.439640
62	1	0	3.262765	-1.858167	2.866053
63	1	0	1.883214	-0.782099	3.210508
64	1	0	3.170942	-0.240549	2.124700
65	6	0	-0.135978	-2.747243	-2.853879
66	1	0	-0.700144	-2.743670	-3.793881
67	1	0	0.443488	-3.677276	-2.871947
68	7	0	2.304659	1.142550	-0.227259
69	7	0	1.619684	-1.128534	-1.777978
70	7	0	1.851811	-1.651005	1.270271
71	8	0	0.582897	1.552495	1.750093
72	8	0	1.920519	3.112573	2.698775
73	60	0	0.000000	0.047614	-0.000002

E(RTPSSh) = -1675.59950314

Zero-point correction= 0.619624 (Hartree/Particle)

Thermal correction to Energy= 0.653028

Thermal correction to Enthalpy= 0.653972

Thermal correction to Gibbs Free Energy= 0.558844

Sum of electronic and zero-point Energies= -1674.979879

Sum of electronic and thermal Energies= -1674.946475

Sum of electronic and thermal Enthalpies= -1674.945531

Sum of electronic and thermal Free Energies= -1675.040659

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.361478	-2.488041	1.673704
2	6	0	-2.443887	-2.245460	0.631462
3	6	0	-3.626098	-2.982312	0.594937
4	1	0	-3.779721	-3.776267	1.316201
5	6	0	-4.581664	-2.655976	-0.371396
6	1	0	-5.518708	-3.201356	-0.422658
7	6	0	-4.329816	-1.614521	-1.267501

8	1	0	-5.060186	-1.335931	-2.019681
9	6	0	-3.111386	-0.931407	-1.180816
10	6	0	-2.705624	0.140005	-2.169281
11	1	0	-2.175543	-0.361410	-2.987974
12	1	0	-3.594491	0.615711	-2.605870
13	6	0	-2.530165	2.219435	-0.861570
14	1	0	-3.446079	2.503044	-1.400624
15	1	0	-1.909575	3.113186	-0.810987
16	6	0	-2.938731	1.785617	0.550098
17	1	0	-3.517311	2.611577	0.992957
18	1	0	-3.609833	0.926279	0.492396
19	6	0	0.594381	3.388887	-1.453241
20	1	0	1.246978	4.231250	-1.734756
21	1	0	-0.052666	3.767440	-0.658832
22	6	0	-1.067771	1.749136	-2.829266
23	1	0	-1.803559	1.930538	-3.625885
24	1	0	-0.416581	0.942226	-3.182242
25	6	0	-2.454006	0.740758	2.642458
26	1	0	-3.158268	1.421223	3.144616
27	1	0	-1.695588	0.427313	3.359332
28	1	0	-2.999052	-0.142478	2.305125
29	6	0	-0.256438	3.054360	-2.692234
30	1	0	0.380437	3.072594	-3.584303
31	1	0	-0.932331	3.910352	-2.802910
32	7	0	-2.201298	-1.252277	-0.246939
33	7	0	-1.780125	1.183376	-1.628673
34	7	0	-1.824892	1.404822	1.474801
35	8	0	-0.355750	-1.663460	1.616647
36	8	0	-1.504994	-3.409851	2.482785
37	6	0	1.731828	-1.880265	-2.280821
38	6	0	2.727375	-1.860702	-1.129902
39	6	0	3.946663	-2.534539	-1.173861
40	1	0	4.216128	-3.090289	-2.064296
41	6	0	4.783179	-2.464514	-0.056596
42	1	0	5.743542	-2.970295	-0.058390
43	6	0	4.378842	-1.737547	1.066836

44	1	0	5.010170	-1.670742	1.946349
45	6	0	3.137743	-1.093943	1.039060
46	6	0	2.548070	-0.357536	2.221151
47	1	0	1.878982	-1.047009	2.747617
48	1	0	3.335497	-0.049952	2.922602
49	6	0	2.675332	1.875542	1.319310
50	1	0	3.496562	1.357160	0.816255
51	1	0	3.114534	2.408615	2.174716
52	6	0	2.068039	2.900796	0.366571
53	1	0	1.311099	3.492402	0.883567
54	1	0	2.863887	3.601448	0.069723
55	6	0	-1.110219	2.628534	1.932543
56	1	0	-1.838423	3.338301	2.357949
57	1	0	-0.702379	3.117273	1.045584
58	6	0	0.936093	1.215293	3.013239
59	1	0	1.634765	1.383055	3.847245
60	1	0	0.352984	0.323579	3.262239
61	6	0	2.465576	1.895260	-1.820269
62	1	0	3.052974	2.761276	-2.160625
63	1	0	1.990874	1.423734	-2.683612
64	1	0	3.140225	1.170804	-1.361139
65	6	0	0.005435	2.443047	2.987306
66	1	0	-0.460425	2.425778	3.979803
67	1	0	0.601052	3.363040	2.970602
68	7	0	2.349475	-1.154921	-0.047709
69	7	0	1.729514	0.825563	1.802569
70	7	0	1.427578	2.312998	-0.846403
71	8	0	0.623529	-1.234897	-2.049813
72	8	0	2.021809	-2.486497	-3.316216
73	60	0	0.037231	-0.033537	-0.073373

E(RTPSSh) = -1675.59395789

Zero-point correction= 0.618881 (Hartree/Particle)

Thermal correction to Energy= 0.652557

Thermal correction to Enthalpy= 0.653502

Thermal correction to Gibbs Free Energy= 0.557851

Sum of electronic and zero-point Energies= -1674.975077

Sum of electronic and thermal Energies= -1674.941401

Sum of electronic and thermal Enthalpies= -1674.940456

Sum of electronic and thermal Free Energies= -1675.036107

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.730399	-1.882115	-2.279903
2	6	0	2.726225	-1.862013	-1.129238
3	6	0	3.945553	-2.535784	-1.173278
4	1	0	4.214607	-3.092245	-2.063393
5	6	0	4.782698	-2.464646	-0.056557
6	1	0	5.743116	-2.970332	-0.058436
7	6	0	4.378948	-1.736637	1.066418
8	1	0	5.010879	-1.668773	1.945420
9	6	0	3.137686	-1.093351	1.038861
10	6	0	2.548645	-0.356063	2.220704
11	1	0	1.879852	-1.045115	2.748066
12	1	0	3.336467	-0.048039	2.921535
13	6	0	2.675412	1.876631	1.318129
14	1	0	3.496689	1.358221	0.815115
15	1	0	3.114607	2.409883	2.173425
16	6	0	2.067808	2.901604	0.365212
17	1	0	1.310831	3.493151	0.882246
18	1	0	2.863470	3.602360	0.068103
19	6	0	-1.110236	2.629596	1.931986
20	1	0	-1.838507	3.339179	2.357580
21	1	0	-0.702966	3.118299	1.044746
22	6	0	0.936420	1.216700	3.012370
23	1	0	1.635151	1.384562	3.846337
24	1	0	0.353293	0.325054	3.261654
25	6	0	2.465241	1.894736	-1.820996
26	1	0	3.053503	2.760223	-2.161244

27	1	0	1.990470	1.423563	-2.684499
28	1	0	3.139160	1.169714	-1.361659
29	6	0	0.005852	2.444505	2.986363
30	1	0	-0.459633	2.427530	3.979048
31	1	0	0.601524	3.364445	2.969232
32	7	0	2.348742	-1.155526	-0.047376
33	7	0	1.729812	0.826667	1.801758
34	7	0	1.427297	2.313398	-0.847459
35	8	0	0.622087	-1.236659	-2.049070
36	8	0	2.020163	-2.488922	-3.315031
37	6	0	-1.360092	-2.488125	1.674205
38	6	0	-2.442997	-2.245777	0.632415
39	6	0	-3.625170	-2.982708	0.596448
40	1	0	-3.778466	-3.776557	1.317902
41	6	0	-4.581091	-2.656582	-0.369594
42	1	0	-5.518126	-3.202024	-0.420444
43	6	0	-4.329615	-1.615243	-1.265952
44	1	0	-5.060281	-1.336826	-2.017915
45	6	0	-3.111225	-0.931985	-1.179785
46	6	0	-2.706046	0.139336	-2.168603
47	1	0	-2.176244	-0.362146	-2.987428
48	1	0	-3.595215	0.614772	-2.604868
49	6	0	-2.530204	2.219366	-0.861799
50	1	0	-3.446156	2.503011	-1.400770
51	1	0	-1.909434	3.113020	-0.811527
52	6	0	-2.938601	1.785842	0.549976
53	1	0	-3.517401	2.611695	0.992747
54	1	0	-3.609450	0.926281	0.492526
55	6	0	0.594208	3.388972	-1.454842
56	1	0	1.246833	4.231031	-1.737221
57	1	0	-0.052553	3.768235	-0.660527
58	6	0	-1.068152	1.748172	-2.829574
59	1	0	-1.803983	1.929050	-3.626278
60	1	0	-0.416933	0.941128	-3.182222
61	6	0	-2.453548	0.741641	2.642555
62	1	0	-3.158441	1.421848	3.144183

63	1	0	-1.695128	0.429151	3.359851
64	1	0	-2.997825	-0.142164	2.305471
65	6	0	-0.257042	3.053614	-2.693355
66	1	0	0.379521	3.071527	-3.585664
67	1	0	-0.933145	3.909413	-2.804254
68	7	0	-2.200778	-1.252689	-0.246175
69	7	0	-1.780464	1.182988	-1.628655
70	7	0	-1.824575	1.405601	1.474748
71	8	0	-0.354298	-1.663721	1.616303
72	8	0	-1.503354	-3.409588	2.483740
73	60	0	0.037274	-0.033203	-0.073421

E(RTPSSh) = -1675.59395966

Zero-point correction= 0.618887 (Hartree/Particle)

Thermal correction to Energy= 0.652560

Thermal correction to Enthalpy= 0.653504

Thermal correction to Gibbs Free Energy= 0.557869

Sum of electronic and zero-point Energies= -1674.975073

Sum of electronic and thermal Energies= -1674.941400

Sum of electronic and thermal Enthalpies= -1674.940456

Sum of electronic and thermal Free Energies= -1675.036091

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.437922	-2.063431	2.205309
2	6	0	-2.473074	-2.095973	1.090133
3	6	0	-3.607969	-2.903656	1.131166
4	1	0	-3.773002	-3.547166	1.987316
5	6	0	-4.501655	-2.844528	0.058149
6	1	0	-5.400843	-3.452452	0.060383
7	6	0	-4.238507	-1.991979	-1.017597
8	1	0	-4.922143	-1.925078	-1.857133
9	6	0	-3.072093	-1.221110	-0.993593

10	6	0	-2.636523	-0.319233	-2.127225
11	1	0	-1.955015	-0.885456	-2.771641
12	1	0	-3.499293	-0.012823	-2.734691
13	6	0	-2.863506	1.775768	-0.947664
14	1	0	-3.428736	2.364958	-1.683733
15	1	0	-3.583642	1.124370	-0.445061
16	6	0	-2.258354	2.736359	0.074321
17	1	0	-1.641812	3.476224	-0.433815
18	1	0	-3.085048	3.291250	0.543517
19	6	0	0.603827	3.168182	-1.759319
20	1	0	1.280830	3.898336	-2.230422
21	1	0	0.125645	3.697019	-0.935845
22	6	0	-1.217722	1.453515	-2.854324
23	1	0	-1.974304	1.566548	-3.645844
24	1	0	-0.530833	0.667226	-3.182311
25	6	0	-2.311635	1.495278	2.164963
26	1	0	-2.945632	2.271702	2.618225
27	1	0	-1.712922	1.021660	2.944236
28	1	0	-2.951114	0.735543	1.711851
29	6	0	-0.467825	2.799427	-2.812171
30	1	0	-0.011051	2.853041	-3.807364
31	1	0	-1.194147	3.620655	-2.786906
32	7	0	-2.224610	-1.281277	0.047313
33	7	0	-1.887785	0.882229	-1.638908
34	7	0	-1.420796	2.088318	1.134478
35	8	0	-0.443577	-1.248005	1.998777
36	8	0	-1.600728	-2.781151	3.196727
37	6	0	1.438233	-2.064689	-2.204322
38	6	0	2.473533	-2.096309	-1.089246
39	6	0	3.609213	-2.902876	-1.130395
40	1	0	3.774667	-3.546455	-1.986414
41	6	0	4.503238	-2.842458	-0.057732
42	1	0	5.403065	-3.449433	-0.060124
43	6	0	4.239648	-1.989770	1.017803
44	1	0	4.923585	-1.921780	1.857003
45	6	0	3.072356	-1.220217	0.994035

46	6	0	2.636333	-0.318239	2.127379
47	1	0	1.954691	-0.884353	2.771730
48	1	0	3.498874	-0.011458	2.734964
49	6	0	2.862993	1.776655	0.947289
50	1	0	3.583509	1.125320	0.445132
51	1	0	3.427801	2.366331	1.683249
52	6	0	2.257798	2.736755	-0.075181
53	1	0	1.641424	3.476952	0.432667
54	1	0	3.084486	3.291316	-0.544761
55	6	0	-0.604420	3.168401	1.758213
56	1	0	-1.281269	3.899097	2.228701
57	1	0	-0.125977	3.696508	0.934442
58	6	0	1.217048	1.454334	2.853869
59	1	0	1.973516	1.567544	3.645463
60	1	0	0.530251	0.667926	3.181760
61	6	0	2.310775	1.494627	-2.165205
62	1	0	2.944719	2.270771	-2.619010
63	1	0	1.712004	1.020500	-2.944128
64	1	0	2.950336	0.735200	-1.711679
65	6	0	0.466891	2.800076	2.811449
66	1	0	0.009783	2.853648	3.806498
67	1	0	1.192991	3.621509	2.786332
68	7	0	2.224529	-1.281677	-0.046517
69	7	0	1.887426	0.883022	1.638603
70	7	0	1.420018	2.088325	-1.134982
71	8	0	0.443818	-1.249220	-1.998217
72	8	0	1.601064	-2.782964	-3.195324
73	60	0	0.000074	-0.010267	-0.000147

E(RTPSSh) = -1675.58772159

Zero-point correction= 0.618161 (Hartree/Particle)

Thermal correction to Energy= 0.652329

Thermal correction to Enthalpy= 0.653273

Thermal correction to Gibbs Free Energy= 0.556193

Sum of electronic and zero-point Energies= -1674.969561

Sum of electronic and thermal Energies= -1674.935393

Sum of electronic and thermal Enthalpies= -1674.934449

Sum of electronic and thermal Free Energies= -1675.031529

[Eu(Me$_2$tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.511394	-2.230433	-1.851646
2	6	0	2.537089	-2.049280	-0.742717
3	6	0	3.738397	-2.753537	-0.701676
4	1	0	3.957989	-3.478227	-1.476809
5	6	0	4.627477	-2.485902	0.343559
6	1	0	5.577259	-3.007985	0.402729
7	6	0	4.291980	-1.535573	1.310753
8	1	0	4.968528	-1.307301	2.127471
9	6	0	3.059791	-0.878888	1.210288
10	6	0	2.559857	0.085395	2.263793
11	1	0	2.025018	-0.511101	3.011667
12	1	0	3.402123	0.568740	2.777150
13	6	0	2.314165	2.275222	1.161896
14	1	0	3.146437	2.590212	1.808281
15	1	0	1.616733	3.113708	1.115284
16	6	0	2.870527	1.987994	-0.232254
17	1	0	3.437487	2.873909	-0.557974
18	1	0	3.579438	1.158327	-0.189515
19	6	0	-1.126391	2.882224	1.676364
20	1	0	-1.864377	3.650451	1.957611
21	1	0	-0.603905	3.269389	0.797479
22	6	0	0.795865	1.531702	2.972513
23	1	0	1.483747	1.749637	3.802606
24	1	0	0.225399	0.641004	3.254248
25	6	0	2.570418	1.086556	-2.429494

26	1	0	3.250455	1.837098	-2.859861
27	1	0	1.868399	0.761412	-3.197006
28	1	0	3.157846	0.223789	-2.111455
29	6	0	-0.143143	2.744254	2.853769
30	1	0	-0.710145	2.741504	3.792086
31	1	0	0.439350	3.672338	2.873874
32	7	0	2.217292	-1.140059	0.199030
33	7	0	1.597094	1.119275	1.770782
34	7	0	1.842050	1.641634	-1.261560
35	8	0	0.464402	-1.460896	-1.751745
36	8	0	1.728060	-3.055479	-2.743818
37	6	0	-1.511175	-2.230775	1.851362
38	6	0	-2.537003	-2.049405	0.742592
39	6	0	-3.738320	-2.753646	0.701559
40	1	0	-3.957863	-3.478420	1.476628
41	6	0	-4.627452	-2.485920	-0.343608
42	1	0	-5.577238	-3.007997	-0.402774
43	6	0	-4.291988	-1.535532	-1.310755
44	1	0	-4.968568	-1.307201	-2.127430
45	6	0	-3.059790	-0.878861	-1.210299
46	6	0	-2.559879	0.085468	-2.263777
47	1	0	-2.025060	-0.510998	-3.011689
48	1	0	-3.402158	0.568832	-2.777094
49	6	0	-2.314176	2.275251	-1.161810
50	1	0	-3.146442	2.590273	-1.808186
51	1	0	-1.616742	3.113734	-1.115152
52	6	0	-2.870554	1.987950	0.232319
53	1	0	-3.437523	2.873845	0.558078
54	1	0	-3.579460	1.158281	0.189529
55	6	0	1.126317	2.882328	-1.676211
56	1	0	1.864279	3.650599	-1.957400
57	1	0	0.603816	3.269403	-0.797296
58	6	0	-0.795881	1.531824	-2.972452
59	1	0	-1.483760	1.749775	-3.802544
60	1	0	-0.225379	0.641159	-3.254219
61	6	0	-2.570494	1.086376	2.429494

62	1	0	-3.250538	1.836889	2.859898
63	1	0	-1.868501	0.761168	3.197002
64	1	0	-3.157920	0.223640	2.111372
65	6	0	0.143083	2.744401	-2.853633
66	1	0	0.710092	2.741723	-3.791946
67	1	0	-0.439440	3.672467	-2.873685
68	7	0	-2.217258	-1.140094	-0.199084
69	7	0	-1.597108	1.119331	-1.770743
70	7	0	-1.842092	1.641539	1.261620
71	8	0	-0.464369	-1.460960	1.751678
72	8	0	-1.728116	-3.055409	2.743850
73	63	0	0.000005	0.008910	-0.000009

E(RTPSSh) = -1677.42096553

Zero-point correction= 0.620293 (Hartree/Particle)

Thermal correction to Energy= 0.653472

Thermal correction to Enthalpy= 0.654417

Thermal correction to Gibbs Free Energy= 0.560112

Sum of electronic and zero-point Energies= -1676.800672

Sum of electronic and thermal Energies= -1676.767493

Sum of electronic and thermal Enthalpies= -1676.766549

Sum of electronic and thermal Free Energies= -1676.860854

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.265827	-2.483333	1.653999
2	6	0	-2.357307	-2.256941	0.621115
3	6	0	-3.522245	-3.019387	0.575690
4	1	0	-3.657562	-3.826096	1.286426
5	6	0	-4.485636	-2.701133	-0.385811
6	1	0	-5.410660	-3.265975	-0.444030
7	6	0	-4.256249	-1.643202	-1.268285
8	1	0	-4.991772	-1.370765	-2.017692

9	6	0	-3.052818	-0.934990	-1.172434
10	6	0	-2.663673	0.151826	-2.147348
11	1	0	-2.130151	-0.336320	-2.971207
12	1	0	-3.557113	0.626515	-2.575254
13	6	0	-2.499172	2.229263	-0.834121
14	1	0	-3.413863	2.512603	-1.375004
15	1	0	-1.880128	3.123980	-0.778005
16	6	0	-2.908889	1.786301	0.574239
17	1	0	-3.487619	2.606814	1.025923
18	1	0	-3.577806	0.925619	0.509489
19	6	0	0.628454	3.372312	-1.429647
20	1	0	1.306218	4.198117	-1.698862
21	1	0	-0.007018	3.757471	-0.628865
22	6	0	-1.024039	1.753394	-2.797126
23	1	0	-1.753174	1.915104	-3.604005
24	1	0	-0.358233	0.948160	-3.122528
25	6	0	-2.419462	0.714406	2.652965
26	1	0	-3.131036	1.383872	3.158930
27	1	0	-1.660602	0.401186	3.369100
28	1	0	-2.955583	-0.169790	2.304278
29	6	0	-0.232564	3.066253	-2.664948
30	1	0	0.394030	3.099290	-3.563901
31	1	0	-0.916322	3.918270	-2.756340
32	7	0	-2.136114	-1.246299	-0.242700
33	7	0	-1.743335	1.194898	-1.597502
34	7	0	-1.792221	1.397881	1.494699
35	8	0	-0.280689	-1.634548	1.591148
36	8	0	-1.380323	-3.412043	2.459527
37	6	0	1.597071	-1.742122	-2.331705
38	6	0	2.595671	-1.834885	-1.189203
39	6	0	3.770042	-2.581343	-1.261759
40	1	0	4.002919	-3.122602	-2.171259
41	6	0	4.612166	-2.598751	-0.146332
42	1	0	5.539667	-3.162066	-0.169121
43	6	0	4.257554	-1.884291	1.001341
44	1	0	4.895770	-1.883262	1.878437

45	6	0	3.057535	-1.166350	1.001788
46	6	0	2.518356	-0.427644	2.205131
47	1	0	1.842752	-1.103682	2.738891
48	1	0	3.329819	-0.144354	2.889059
49	6	0	2.690779	1.805761	1.318817
50	1	0	3.497380	1.270426	0.809980
51	1	0	3.146652	2.330147	2.170615
52	6	0	2.094411	2.839490	0.371492
53	1	0	1.352574	3.444388	0.895705
54	1	0	2.897905	3.526420	0.064369
55	6	0	-1.083424	2.619280	1.972319
56	1	0	-1.815274	3.314155	2.414733
57	1	0	-0.684749	3.128473	1.092461
58	6	0	0.959147	1.182340	3.032358
59	1	0	1.675238	1.345670	3.852242
60	1	0	0.371289	0.298371	3.295436
61	6	0	2.455072	1.827350	-1.818519
62	1	0	3.072182	2.679711	-2.139609
63	1	0	1.965918	1.389525	-2.690382
64	1	0	3.101446	1.070547	-1.371573
65	6	0	0.041094	2.420364	3.016560
66	1	0	-0.415575	2.406275	4.013316
67	1	0	0.646385	3.333864	2.995226
68	7	0	2.264111	-1.145034	-0.081778
69	7	0	1.723396	0.778207	1.808454
70	7	0	1.430216	2.263256	-0.837568
71	8	0	0.541704	-1.021723	-2.068026
72	8	0	1.832386	-2.329415	-3.390794
73	63	0	0.028616	0.015041	-0.040167

E(RTPSSh) = -1677.41500120

Zero-point correction= 0.618699 (Hartree/Particle)

Thermal correction to Energy= 0.652500

Thermal correction to Enthalpy= 0.653444

Thermal correction to Gibbs Free Energy= 0.557328

Sum of electronic and zero-point Energies= -1676.796302

Sum of electronic and thermal Energies= -1676.762501

Sum of electronic and thermal Enthalpies= -1676.761557

Sum of electronic and thermal Free Energies= -1676.857673

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.596050	-1.743457	-2.331008
2	6	0	2.594868	-1.835921	-1.188677
3	6	0	3.769038	-2.582699	-1.261128
4	1	0	4.001595	-3.124432	-2.170432
5	6	0	4.611393	-2.599809	-0.145866
6	1	0	5.538760	-3.163353	-0.168597
7	6	0	4.257173	-1.884763	1.001560
8	1	0	4.895558	-1.883496	1.878538
9	6	0	3.057322	-1.166540	1.001929
10	6	0	2.518573	-0.427189	2.205099
11	1	0	1.843111	-1.102927	2.739416
12	1	0	3.330307	-0.143719	2.888641
13	6	0	2.691224	1.805939	1.318321
14	1	0	3.497939	1.270452	0.809816
15	1	0	3.147042	2.330538	2.170046
16	6	0	2.095033	2.839319	0.370517
17	1	0	1.353101	3.444401	0.894386
18	1	0	2.898561	3.526129	0.063227
19	6	0	-1.083159	2.620330	1.972026
20	1	0	-1.815027	3.314981	2.414765
21	1	0	-0.684854	3.129799	1.092148
22	6	0	0.959340	1.183035	3.031887
23	1	0	1.675356	1.346197	3.851865
24	1	0	0.371213	0.299232	3.294935
25	6	0	2.455964	1.826239	-1.819044
26	1	0	3.073364	2.678359	-2.140215
27	1	0	1.966890	1.388324	-2.690916

28	1	0	3.102025	1.069369	-1.371748
29	6	0	0.041705	2.421359	3.015925
30	1	0	-0.414646	2.407712	4.012838
31	1	0	0.647330	3.334626	2.994166
32	7	0	2.263696	-1.145473	-0.081499
33	7	0	1.723725	0.778569	1.808127
34	7	0	1.430990	2.262642	-0.838453
35	8	0	0.540873	-1.022742	-2.067471
36	8	0	1.831063	-2.331258	-3.389893
37	6	0	-1.266283	-2.482635	1.654727
38	6	0	-2.357686	-2.256424	0.621726
39	6	0	-3.522681	-3.018795	0.576402
40	1	0	-3.658102	-3.825333	1.287319
41	6	0	-4.485974	-2.700689	-0.385240
42	1	0	-5.411028	-3.265495	-0.443437
43	6	0	-4.256454	-1.642943	-1.267907
44	1	0	-4.991918	-1.370615	-2.017422
45	6	0	-3.052992	-0.934782	-1.172115
46	6	0	-2.663722	0.151783	-2.147255
47	1	0	-2.130493	-0.336654	-2.971131
48	1	0	-3.557096	0.626667	-2.575076
49	6	0	-2.498357	2.229636	-0.834790
50	1	0	-3.412834	2.513331	-1.375848
51	1	0	-1.878838	3.124032	-0.778838
52	6	0	-2.908394	1.787238	0.573645
53	1	0	-3.487048	2.607970	1.025024
54	1	0	-3.577450	0.926643	0.509077
55	6	0	0.629496	3.371643	-1.431028
56	1	0	1.307451	4.197158	-1.700636
57	1	0	-0.005854	3.757289	-0.630375
58	6	0	-1.023352	1.752391	-2.797621
59	1	0	-1.752356	1.913794	-3.604676
60	1	0	-0.357670	0.946832	-3.122489
61	6	0	-2.419455	0.715675	2.652641
62	1	0	-3.131173	1.385261	3.158245
63	1	0	-1.660790	0.402664	3.369084

64	1	0	-2.955459	-0.168623	2.304021
65	6	0	-0.231689	3.065191	-2.666111
66	1	0	0.394816	3.097717	-3.565151
67	1	0	-0.915337	3.917264	-2.757820
68	7	0	-2.136348	-1.245980	-0.242277
69	7	0	-1.742967	1.194680	-1.597765
70	7	0	-1.791903	1.398897	1.494384
71	8	0	-0.280787	-1.634328	1.591231
72	8	0	-1.381138	-3.410753	2.460887
73	63	0	0.028591	0.015213	-0.040001

E(RTPSSh) = -1677.41500329

Zero-point correction= 0.618705 (Hartree/Particle)

Thermal correction to Energy= 0.652502

Thermal correction to Enthalpy= 0.653446

Thermal correction to Gibbs Free Energy= 0.557347

Sum of electronic and zero-point Energies= -1676.796299

Sum of electronic and thermal Energies= -1676.762502

Sum of electronic and thermal Enthalpies= -1676.761557

Sum of electronic and thermal Free Energies= -1676.857656

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.596294	-1.742260	-2.331612
2	6	0	2.595136	-1.835128	-1.189319
3	6	0	3.769240	-2.581997	-1.261988
4	1	0	4.001767	-3.123437	-2.171474
5	6	0	4.611536	-2.599606	-0.146693
6	1	0	5.538845	-3.163237	-0.169580
7	6	0	4.257313	-1.884983	1.001003
8	1	0	4.895635	-1.884158	1.878027
9	6	0	3.057535	-1.166649	1.001578
10	6	0	2.518640	-0.427858	2.205017

11	1	0	1.843159	-1.103853	2.738992
12	1	0	3.330279	-0.144571	2.888747
13	6	0	2.691358	1.805231	1.318440
14	1	0	3.147880	2.329261	2.170139
15	1	0	3.497477	1.269435	0.809322
16	6	0	2.095148	2.839150	0.371265
17	1	0	1.353470	3.444185	0.895546
18	1	0	2.898761	3.525916	0.064071
19	6	0	-1.083020	2.619567	1.972456
20	1	0	-1.814802	3.314366	2.415099
21	1	0	-0.684473	3.128959	1.092652
22	6	0	0.959598	1.182354	3.032286
23	1	0	1.675755	1.345655	3.852117
24	1	0	0.371682	0.298450	3.295482
25	6	0	2.455431	1.826885	-1.818761
26	1	0	3.072799	2.679078	-2.139828
27	1	0	1.966099	1.389272	-2.690632
28	1	0	3.101582	1.069834	-1.371913
29	6	0	0.041655	2.420468	3.016521
30	1	0	-0.414876	2.406443	4.013343
31	1	0	0.647056	3.333892	2.995099
32	7	0	2.263987	-1.145058	-0.081902
33	7	0	1.723763	0.778002	1.808355
34	7	0	1.430753	2.263034	-0.837757
35	8	0	0.541265	-1.021425	-2.067870
36	8	0	1.831160	-2.329917	-3.390607
37	6	0	-1.266146	-2.483872	1.653433
38	6	0	-2.357704	-2.256971	0.620764
39	6	0	-3.523119	-3.018725	0.575673
40	1	0	-3.658703	-3.825402	1.286401
41	6	0	-4.486658	-2.699783	-0.385445
42	1	0	-5.412071	-3.264030	-0.443367
43	6	0	-4.256929	-1.641904	-1.267900
44	1	0	-4.992585	-1.368901	-2.016977
45	6	0	-3.053011	-0.934478	-1.172448
46	6	0	-2.663519	0.152219	-2.147334

47	1	0	-2.129973	-0.336005	-2.971117
48	1	0	-3.556786	0.627192	-2.575280
49	6	0	-2.498633	2.229742	-0.834124
50	1	0	-3.413157	2.513384	-1.375125
51	1	0	-1.879237	3.124228	-0.777893
52	6	0	-2.908546	1.786834	0.574205
53	1	0	-3.487196	2.607415	1.025887
54	1	0	-3.577581	0.926239	0.509417
55	6	0	0.629235	3.372264	-1.429800
56	1	0	1.307182	4.197877	-1.699154
57	1	0	-0.006056	3.757646	-0.628972
58	6	0	-1.023498	1.753397	-2.796987
59	1	0	-1.752527	1.915028	-3.603993
60	1	0	-0.357690	0.948085	-3.122190
61	6	0	-2.419309	0.714796	2.652945
62	1	0	-3.130870	1.384293	3.158891
63	1	0	-1.660486	0.401535	3.369109
64	1	0	-2.955440	-0.169380	2.304209
65	6	0	-0.232026	3.066267	-2.664958
66	1	0	0.394395	3.099276	-3.564037
67	1	0	-0.915799	3.918287	-2.756234
68	7	0	-2.136139	-1.246453	-0.243087
69	7	0	-1.742996	1.195126	-1.597376
70	7	0	-1.791970	1.398257	1.494717
71	8	0	-0.280882	-1.635209	1.590613
72	8	0	-1.380661	-3.412727	2.458777
73	63	0	0.028597	0.015109	-0.039715

E(RTPSSh) = -1677.41500178

Zero-point correction= 0.618699 (Hartree/Particle)

Thermal correction to Energy= 0.652499

Thermal correction to Enthalpy= 0.653443

Thermal correction to Gibbs Free Energy= 0.557333

Sum of electronic and zero-point Energies= -1676.796303

Sum of electronic and thermal Energies= -1676.762503

Sum of electronic and thermal Enthalpies= -1676.761559

Sum of electronic and thermal Free Energies= -1676.857669

[Gd(Me$_2$tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.461741	-2.208354	-1.862926
2	6	0	2.492878	-2.050640	-0.756235
3	6	0	3.680498	-2.777646	-0.718706
4	1	0	3.885444	-3.504120	-1.496214
5	6	0	4.575529	-2.529921	0.326404
6	1	0	5.515325	-3.070032	0.383264
7	6	0	4.258668	-1.576375	1.296700
8	1	0	4.939906	-1.363169	2.113643
9	6	0	3.038776	-0.896343	1.199217
10	6	0	2.556616	0.073559	2.255620
11	1	0	2.023401	-0.517536	3.008626
12	1	0	3.406864	0.551497	2.760773
13	6	0	2.319265	2.268272	1.161045
14	1	0	3.152969	2.579247	1.807429
15	1	0	1.624756	3.109303	1.115245
16	6	0	2.873523	1.977768	-0.233454
17	1	0	3.441549	2.861680	-0.562434
18	1	0	3.580509	1.146464	-0.189594
19	6	0	-1.126868	2.871919	1.674530
20	1	0	-1.865052	3.640172	1.954989
21	1	0	-0.604550	3.258349	0.794641
22	6	0	0.799756	1.526720	2.971227
23	1	0	1.489662	1.748143	3.798719
24	1	0	0.231851	0.635461	3.255510
25	6	0	2.567541	1.073684	-2.429689
26	1	0	3.245115	1.824262	-2.863675

27	1	0	1.862921	0.745850	-3.193572
28	1	0	3.157312	0.212539	-2.111668
29	6	0	-0.142743	2.736735	2.851714
30	1	0	-0.709513	2.733392	3.790175
31	1	0	0.436895	3.666660	2.870458
32	7	0	2.191033	-1.138078	0.188012
33	7	0	1.597894	1.113301	1.767841
34	7	0	1.842555	1.630437	-1.260638
35	8	0	0.429510	-1.420769	-1.756174
36	8	0	1.660797	-3.032902	-2.760019
37	6	0	-1.461663	-2.208453	1.862855
38	6	0	-2.492849	-2.050676	0.756218
39	6	0	-3.680469	-2.777682	0.718698
40	1	0	-3.885395	-3.504179	1.496190
41	6	0	-4.575518	-2.529940	-0.326393
42	1	0	-5.515312	-3.070055	-0.383250
43	6	0	-4.258671	-1.576382	-1.296682
44	1	0	-4.939918	-1.363171	-2.113616
45	6	0	-3.038779	-0.896349	-1.199207
46	6	0	-2.556631	0.073557	-2.255612
47	1	0	-2.023425	-0.517533	-3.008628
48	1	0	-3.406884	0.551497	-2.760752
49	6	0	-2.319272	2.268270	-1.161045
50	1	0	-3.152976	2.579245	-1.807428
51	1	0	-1.624762	3.109300	-1.115244
52	6	0	-2.873533	1.977765	0.233454
53	1	0	-3.441558	2.861677	0.562435
54	1	0	-3.580518	1.146461	0.189592
55	6	0	1.126857	2.871922	-1.674533
56	1	0	1.865040	3.640173	-1.954995
57	1	0	0.604540	3.258350	-0.794644
58	6	0	-0.799764	1.526713	-2.971224
59	1	0	-1.489668	1.748131	-3.798720
60	1	0	-0.231856	0.635454	-3.255503
61	6	0	-2.567551	1.073685	2.429690
62	1	0	-3.245120	1.824266	2.863677

63	1	0	-1.862932	0.745846	3.193571
64	1	0	-3.157328	0.212543	2.111669
65	6	0	0.142729	2.736731	-2.851715
66	1	0	0.709498	2.733391	-3.790178
67	1	0	-0.436913	3.666653	-2.870458
68	7	0	-2.191025	-1.138090	-0.188012
69	7	0	-1.597904	1.113297	-1.767839
70	7	0	-1.842565	1.630433	1.260637
71	8	0	-0.429510	-1.420756	1.756179
72	8	0	-1.660818	-3.032843	2.760070
73	64	0	0.000000	0.037369	-0.000003

E(RTPSSh) = -1678.01204993

Zero-point correction= 0.620225 (Hartree/Particle)

Thermal correction to Energy= 0.653393

Thermal correction to Enthalpy= 0.654337

Thermal correction to Gibbs Free Energy= 0.560111

Sum of electronic and zero-point Energies= -1677.391825

Sum of electronic and thermal Energies= -1677.358657

Sum of electronic and thermal Enthalpies= -1677.357713

Sum of electronic and thermal Free Energies= -1677.451939

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.252412	-2.465975	1.659926
2	6	0	-2.341065	-2.248941	0.622663
3	6	0	-3.503073	-3.015646	0.575663
4	1	0	-3.638067	-3.820674	1.288376
5	6	0	-4.464649	-2.703102	-0.389595
6	1	0	-5.387657	-3.271113	-0.449157
7	6	0	-4.236252	-1.646348	-1.273669
8	1	0	-4.970526	-1.377693	-2.025686
9	6	0	-3.035636	-0.933634	-1.175636

10	6	0	-2.647545	0.153987	-2.149291
11	1	0	-2.113924	-0.333044	-2.973625
12	1	0	-3.541007	0.629810	-2.575932
13	6	0	-2.480883	2.229540	-0.832467
14	1	0	-3.391561	2.519839	-1.376546
15	1	0	-1.857222	3.120570	-0.770131
16	6	0	-2.900628	1.784832	0.572939
17	1	0	-3.482301	2.605366	1.020823
18	1	0	-3.569742	0.924719	0.502662
19	6	0	0.644629	3.374866	-1.436293
20	1	0	1.322489	4.200430	-1.706472
21	1	0	0.011411	3.759231	-0.633234
22	6	0	-1.009187	1.755077	-2.798164
23	1	0	-1.740205	1.915084	-3.603704
24	1	0	-0.342766	0.950431	-3.123264
25	6	0	-2.422789	0.707866	2.653502
26	1	0	-3.139117	1.374681	3.156362
27	1	0	-1.666832	0.396080	3.373460
28	1	0	-2.954597	-0.177208	2.300512
29	6	0	-0.220115	3.069379	-2.668753
30	1	0	0.403308	3.103322	-3.569945
31	1	0	-0.905476	3.920385	-2.757643
32	7	0	-2.120539	-1.239714	-0.242878
33	7	0	-1.726613	1.195215	-1.597597
34	7	0	-1.790555	1.395630	1.501088
35	8	0	-0.272610	-1.611370	1.597980
36	8	0	-1.364291	-3.392457	2.468585
37	6	0	1.558370	-1.741977	-2.329561
38	6	0	2.561637	-1.845676	-1.192549
39	6	0	3.724684	-2.609312	-1.267582
40	1	0	3.946146	-3.156525	-2.176376
41	6	0	4.570269	-2.636590	-0.154917
42	1	0	5.489110	-3.213874	-0.179270
43	6	0	4.229753	-1.914810	0.992343
44	1	0	4.870429	-1.921825	1.867651
45	6	0	3.040075	-1.179804	0.995482

46	6	0	2.514342	-0.434379	2.200321
47	1	0	1.839594	-1.105633	2.740815
48	1	0	3.332220	-0.152740	2.877269
49	6	0	2.694583	1.797165	1.314646
50	1	0	3.498880	1.257676	0.806474
51	1	0	3.152763	2.319192	2.166722
52	6	0	2.105062	2.834562	0.366863
53	1	0	1.361256	3.438488	0.889730
54	1	0	2.911664	3.521004	0.066615
55	6	0	-1.089833	2.618531	1.988037
56	1	0	-1.825625	3.301516	2.442174
57	1	0	-0.701721	3.140035	1.110285
58	6	0	0.961264	1.179200	3.030946
59	1	0	1.679852	1.339857	3.849190
60	1	0	0.372014	0.296170	3.293569
61	6	0	2.470728	1.826622	-1.825480
62	1	0	3.093770	2.676256	-2.142687
63	1	0	1.982144	1.393222	-2.699901
64	1	0	3.111153	1.064844	-1.378145
65	6	0	0.045047	2.418908	3.021435
66	1	0	-0.402138	2.405200	4.022544
67	1	0	0.651380	3.331565	2.994563
68	7	0	2.243753	-1.148659	-0.085626
69	7	0	1.722680	0.773573	1.805099
70	7	0	1.445221	2.264502	-0.847383
71	8	0	0.513626	-1.008398	-2.060920
72	8	0	1.779983	-2.333792	-3.389216
73	64	0	0.028615	0.022869	-0.035832

E(RTPSSh) = -1678.00575012

Zero-point correction= 0.618801 (Hartree/Particle)

Thermal correction to Energy= 0.652488

Thermal correction to Enthalpy= 0.653433

Thermal correction to Gibbs Free Energy= 0.557918

Sum of electronic and zero-point Energies= -1677.386949

Sum of electronic and thermal Energies= -1677.353262

Sum of electronic and thermal Enthalpies= -1677.352318

Sum of electronic and thermal Free Energies= -1677.447832

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.557884	-1.742146	-2.329421
2	6	0	2.561168	-1.845899	-1.192456
3	6	0	3.724232	-2.609501	-1.267589
4	1	0	3.945606	-3.156748	-2.176385
5	6	0	4.569973	-2.636661	-0.155037
6	1	0	5.488823	-3.213937	-0.179471
7	6	0	4.229621	-1.914763	0.992196
8	1	0	4.870443	-1.921649	1.867400
9	6	0	3.039918	-1.179797	0.995444
10	6	0	2.514374	-0.434205	2.200292
11	1	0	1.839646	-1.105330	2.740942
12	1	0	3.332415	-0.152572	2.877066
13	6	0	2.694801	1.797225	1.314196
14	1	0	3.498985	1.257436	0.806147
15	1	0	3.153008	2.319527	2.166078
16	6	0	2.105267	2.834360	0.366075
17	1	0	1.361676	3.438630	0.888845
18	1	0	2.911975	3.520477	0.065394
19	6	0	-1.089379	2.618897	1.987581
20	1	0	-1.825077	3.302160	2.441436
21	1	0	-0.701205	3.140117	1.109681
22	6	0	0.961507	1.179721	3.030758
23	1	0	1.680142	1.340370	3.848958
24	1	0	0.372153	0.296799	3.293516
25	6	0	2.470398	1.825687	-1.826037
26	1	0	3.093312	2.675240	-2.143710
27	1	0	1.981636	1.391923	-2.700183
28	1	0	3.110987	1.064126	-1.378542

29	6	0	0.045469	2.419505	3.021007
30	1	0	-0.401680	2.406100	4.022139
31	1	0	0.651837	3.332139	2.993862
32	7	0	2.243402	-1.148826	-0.085529
33	7	0	1.722871	0.773783	1.804976
34	7	0	1.445090	2.263915	-0.847843
35	8	0	0.512994	-1.008810	-2.060717
36	8	0	1.779641	-2.333750	-3.389183
37	6	0	-1.251895	-2.465849	1.660157
38	6	0	-2.340720	-2.249036	0.623028
39	6	0	-3.502610	-3.015958	0.576228
40	1	0	-3.637286	-3.821057	1.288924
41	6	0	-4.464447	-2.703504	-0.388781
42	1	0	-5.387424	-3.271597	-0.448136
43	6	0	-4.236357	-1.646710	-1.272908
44	1	0	-4.970861	-1.378104	-2.024724
45	6	0	-3.035780	-0.933915	-1.175188
46	6	0	-2.647918	0.153630	-2.149001
47	1	0	-2.114441	-0.333481	-2.973384
48	1	0	-3.541444	0.629425	-2.575528
49	6	0	-2.481014	2.229423	-0.832515
50	1	0	-3.391724	2.519648	-1.376558
51	1	0	-1.857301	3.120443	-0.770429
52	6	0	-2.900526	1.784947	0.573013
53	1	0	-3.482112	2.605530	1.020923
54	1	0	-3.569615	0.924787	0.503038
55	6	0	0.644558	3.374303	-1.436886
56	1	0	1.322524	4.199714	-1.707225
57	1	0	0.011464	3.758857	-0.633820
58	6	0	-1.009551	1.754508	-2.798329
59	1	0	-1.740664	1.914416	-3.603804
60	1	0	-0.343239	0.949728	-3.123337
61	6	0	-2.422494	0.708456	2.653694
62	1	0	-3.138959	1.375371	3.156234
63	1	0	-1.666559	0.397060	3.373830
64	1	0	-2.954111	-0.176836	2.300968

65	6	0	-0.220354	3.068754	-2.669206
66	1	0	0.402946	3.102559	-3.570491
67	1	0	-0.905647	3.919821	-2.758072
68	7	0	-2.120460	-1.239830	-0.242571
69	7	0	-1.726854	1.194890	-1.597557
70	7	0	-1.790276	1.395892	1.501065
71	8	0	-0.272936	-1.610272	1.598917
72	8	0	-1.362912	-3.393118	2.468056
73	64	0	0.028630	0.023264	-0.035747

E(RTPSSh) = -1678.00575129

Zero-point correction= 0.618802 (Hartree/Particle)

Thermal correction to Energy= 0.652490

Thermal correction to Enthalpy= 0.653434

Thermal correction to Gibbs Free Energy= 0.557916

Sum of electronic and zero-point Energies= -1677.386949

Sum of electronic and thermal Energies= -1677.353261

Sum of electronic and thermal Enthalpies= -1677.352317

Sum of electronic and thermal Free Energies= -1677.447835

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.301465	-2.014495	2.221892
2	6	0	-2.355576	-2.094052	1.131222
3	6	0	-3.461969	-2.937966	1.196148
4	1	0	-3.591439	-3.581796	2.058179
5	6	0	-4.374774	-2.913691	0.137594
6	1	0	-5.253669	-3.550305	0.157351
7	6	0	-4.156500	-2.058370	-0.945488
8	1	0	-4.855030	-2.017422	-1.774359
9	6	0	-3.015993	-1.249029	-0.943752
10	6	0	-2.629341	-0.336037	-2.082622
11	1	0	-1.956851	-0.887135	-2.748283

12	1	0	-3.514164	-0.035760	-2.660573
13	6	0	-2.862958	1.745121	-0.889602
14	1	0	-3.453073	2.325550	-1.612925
15	1	0	-3.561634	1.081434	-0.372651
16	6	0	-2.248976	2.710541	0.119400
17	1	0	-1.651826	3.458440	-0.400288
18	1	0	-3.069366	3.254944	0.610829
19	6	0	0.570367	3.159199	-1.766081
20	1	0	1.252366	3.880538	-2.243049
21	1	0	0.112304	3.691551	-0.933442
22	6	0	-1.264169	1.459085	-2.834829
23	1	0	-2.050445	1.574736	-3.596510
24	1	0	-0.584043	0.681030	-3.191842
25	6	0	-2.246027	1.467796	2.208177
26	1	0	-2.877334	2.241214	2.669820
27	1	0	-1.628020	1.002226	2.976634
28	1	0	-2.887348	0.700939	1.770200
29	6	0	-0.522059	2.807260	-2.800665
30	1	0	-0.087840	2.873841	-3.805090
31	1	0	-1.250004	3.625776	-2.748778
32	7	0	-2.150024	-1.275351	0.082167
33	7	0	-1.884456	0.870715	-1.602088
34	7	0	-1.380611	2.065920	1.157401
35	8	0	-0.343841	-1.164825	1.980046
36	8	0	-1.413133	-2.723084	3.226419
37	6	0	1.299919	-2.016123	-2.220926
38	6	0	2.354324	-2.095640	-1.130520
39	6	0	3.460950	-2.939227	-1.195809
40	1	0	3.590249	-3.583163	-2.057790
41	6	0	4.374287	-2.914398	-0.137738
42	1	0	5.253429	-3.550660	-0.157846
43	6	0	4.156260	-2.058923	0.945287
44	1	0	4.855240	-2.017506	1.773753
45	6	0	3.015371	-1.250128	0.944054
46	6	0	2.628892	-0.336980	2.082813
47	1	0	1.955644	-0.887503	2.748154

48	1	0	3.513688	-0.037245	2.661096
49	6	0	2.864087	1.743643	0.888979
50	1	0	3.562286	1.079214	0.372306
51	1	0	3.454508	2.323863	1.612134
52	6	0	2.250762	2.709092	-0.120402
53	1	0	1.654342	3.457723	0.399051
54	1	0	3.071522	3.252587	-0.612199
55	6	0	-0.568272	3.160054	1.764790
56	1	0	-1.249625	3.882488	2.241000
57	1	0	-0.109469	3.691209	0.931824
58	6	0	1.265016	1.459381	2.834359
59	1	0	2.051366	1.574808	3.595985
60	1	0	0.584527	0.681754	3.191643
61	6	0	2.246624	1.465305	-2.208491
62	1	0	2.878775	2.237890	-2.670402
63	1	0	1.628252	1.000006	-2.976833
64	1	0	2.887147	0.697974	-1.770148
65	6	0	0.523469	2.807848	2.799894
66	1	0	0.088853	2.874655	3.804139
67	1	0	1.251681	3.626133	2.748192
68	7	0	2.148889	-1.276980	-0.081430
69	7	0	1.884970	0.870264	1.601794
70	7	0	1.381717	2.064722	-1.158054
71	8	0	0.343243	-1.165282	-1.979528
72	8	0	1.410608	-2.725695	-3.224867
73	64	0	-0.000108	0.023382	0.000149

E(RTPSSh) = -1677.99946945

Zero-point correction= 0.619132 (Hartree/Particle)

Thermal correction to Energy= 0.652942

Thermal correction to Enthalpy= 0.653887

Thermal correction to Gibbs Free Energy= 0.558108

Sum of electronic and zero-point Energies= -1677.380337

Sum of electronic and thermal Energies= -1677.346527

Sum of electronic and thermal Enthalpies= -1677.345583

Sum of electronic and thermal Free Energies= -1677.441361

[Ho(Me$_2$tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.401818	-2.178169	1.873928
2	6	0	-2.437260	-2.045271	0.770382
3	6	0	-3.613158	-2.790243	0.734406
4	1	0	-3.808843	-3.515987	1.514992
5	6	0	-4.509320	-2.561005	-0.314124
6	1	0	-5.440798	-3.115338	-0.370584
7	6	0	-4.203938	-1.608166	-1.288761
8	1	0	-4.885692	-1.409570	-2.108921
9	6	0	-2.994720	-0.909278	-1.191593
10	6	0	-2.519200	0.060137	-2.249413
11	1	0	-1.979891	-0.530160	-2.998366
12	1	0	-3.371006	0.532583	-2.756933
13	6	0	-2.299356	2.258845	-1.164002
14	1	0	-3.130451	2.562353	-1.817293
15	1	0	-1.610767	3.104515	-1.115874
16	6	0	-2.857363	1.966407	0.226286
17	1	0	-3.431142	2.846342	0.555529
18	1	0	-3.559069	1.130768	0.181092
19	6	0	1.123314	2.875272	-1.670036
20	1	0	1.871599	3.635758	-1.944361
21	1	0	0.597812	3.266393	-0.794643
22	6	0	-0.783879	1.527376	-2.972285
23	1	0	-1.484520	1.744836	-3.791864
24	1	0	-0.212638	0.640904	-3.262130
25	6	0	-2.549720	1.064221	2.419079
26	1	0	-3.233463	1.811731	2.848461
27	1	0	-1.847547	0.741175	3.186711

28	1	0	-3.133771	0.200075	2.099047
29	6	0	0.148925	2.743304	-2.853913
30	1	0	0.721245	2.743227	-3.788973
31	1	0	-0.435393	3.670201	-2.874674
32	7	0	-2.147054	-1.132112	-0.176737
33	7	0	-1.566627	1.106926	-1.762016
34	7	0	-1.823268	1.625601	1.252063
35	8	0	-0.382927	-1.374637	1.750838
36	8	0	-1.582040	-2.995352	2.780948
37	6	0	1.402071	-2.177587	-1.874503
38	6	0	2.437369	-2.045062	-0.770776
39	6	0	3.613228	-2.790099	-0.734860
40	1	0	3.808940	-3.515692	-1.515580
41	6	0	4.509335	-2.561098	0.313769
42	1	0	5.440783	-3.115488	0.370190
43	6	0	4.203949	-1.608406	1.288547
44	1	0	4.885660	-1.409990	2.108786
45	6	0	2.994762	-0.909457	1.191439
46	6	0	2.519232	0.059786	2.249407
47	1	0	1.979902	-0.530627	2.998254
48	1	0	3.371029	0.532146	2.757024
49	6	0	2.299381	2.258691	1.164389
50	1	0	3.130501	2.562061	1.817713
51	1	0	1.610790	3.104369	1.116468
52	6	0	2.857322	1.966589	-0.225994
53	1	0	3.431072	2.846609	-0.555061
54	1	0	3.559042	1.130950	-0.181035
55	6	0	-1.123525	2.874773	1.670722
56	1	0	-1.871886	3.635099	1.945285
57	1	0	-0.598071	3.266246	0.795458
58	6	0	0.783914	1.526779	2.972568
59	1	0	1.484572	1.744161	3.792153
60	1	0	0.212827	0.640162	3.262271
61	6	0	2.549478	1.065022	-2.419061
62	1	0	3.233169	1.812670	-2.848287
63	1	0	1.847198	0.742232	-3.186705

64	1	0	3.133563	0.200766	-2.099385
65	6	0	-0.149078	2.742600	2.854531
66	1	0	-0.721365	2.742215	3.789610
67	1	0	0.435118	3.669570	2.875521
68	7	0	2.147130	-1.132087	0.176509
69	7	0	1.566658	1.106645	1.762187
70	7	0	1.823159	1.626026	-1.251785
71	8	0	0.383023	-1.374298	-1.751131
72	8	0	1.582021	-2.995038	-2.781335
73	67	0	0.000018	0.038128	-0.000012

E(RTPSSh) = -1679.77332746

Zero-point correction= 0.620915 (Hartree/Particle)

Thermal correction to Energy= 0.653830

Thermal correction to Enthalpy= 0.654774

Thermal correction to Gibbs Free Energy= 0.561410

Sum of electronic and zero-point Energies= -1679.152412

Sum of electronic and thermal Energies= -1679.119498

Sum of electronic and thermal Enthalpies= -1679.118553

Sum of electronic and thermal Free Energies= -1679.211918

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.202311	-2.404191	1.712197
2	6	0	-2.295739	-2.220130	0.676556
3	6	0	-3.446252	-3.003460	0.637136
4	1	0	-3.571746	-3.801460	1.359480
5	6	0	-4.408950	-2.716508	-0.334976
6	1	0	-5.323387	-3.298569	-0.390505
7	6	0	-4.192654	-1.667736	-1.231653
8	1	0	-4.928074	-1.419497	-1.989478
9	6	0	-3.002440	-0.936932	-1.139324
10	6	0	-2.620585	0.141601	-2.123630

11	1	0	-2.076907	-0.351962	-2.937132
12	1	0	-3.515156	0.606565	-2.559406
13	6	0	-2.471605	2.228498	-0.821739
14	1	0	-3.393894	2.496233	-1.357356
15	1	0	-1.862769	3.131112	-0.776260
16	6	0	-2.858880	1.789039	0.591404
17	1	0	-3.420816	2.612995	1.057174
18	1	0	-3.533634	0.932090	0.540680
19	6	0	0.633546	3.373473	-1.429885
20	1	0	1.341787	4.170815	-1.704998
21	1	0	0.012879	3.789764	-0.632799
22	6	0	-1.016803	1.762206	-2.791378
23	1	0	-1.763498	1.921249	-3.582744
24	1	0	-0.352327	0.962337	-3.129680
25	6	0	-2.339510	0.739499	2.668966
26	1	0	-3.012693	1.437082	3.188442
27	1	0	-1.572750	0.401468	3.364028
28	1	0	-2.916864	-0.126456	2.340838
29	6	0	-0.234719	3.079341	-2.662516
30	1	0	0.386794	3.120463	-3.564502
31	1	0	-0.923063	3.928404	-2.744671
32	7	0	-2.086589	-1.218841	-0.200505
33	7	0	-1.707996	1.196145	-1.580557
34	7	0	-1.723810	1.391887	1.485674
35	8	0	-0.235936	-1.535456	1.624532
36	8	0	-1.294860	-3.314689	2.540264
37	6	0	1.425943	-1.737299	-2.338699
38	6	0	2.460764	-1.863705	-1.235702
39	6	0	3.611912	-2.639860	-1.348611
40	1	0	3.800129	-3.185266	-2.265931
41	6	0	4.490803	-2.679869	-0.262366
42	1	0	5.403042	-3.265514	-0.316437
43	6	0	4.191832	-1.958393	0.896284
44	1	0	4.858697	-1.973766	1.751731
45	6	0	3.010777	-1.210546	0.937417
46	6	0	2.531927	-0.459888	2.156352

47	1	0	1.866505	-1.122325	2.717796
48	1	0	3.373002	-0.183776	2.806425
49	6	0	2.718180	1.768393	1.277112
50	1	0	3.505953	1.221428	0.751456
51	1	0	3.198936	2.280629	2.122479
52	6	0	2.122982	2.813156	0.343391
53	1	0	1.424538	3.452875	0.884988
54	1	0	2.937225	3.466634	-0.004946
55	6	0	-0.968607	2.602830	1.918600
56	1	0	-1.674179	3.362723	2.289859
57	1	0	-0.503345	3.027612	1.026272
58	6	0	1.019097	1.167411	3.023954
59	1	0	1.757617	1.331247	3.823425
60	1	0	0.432202	0.288793	3.303889
61	6	0	2.391079	1.762997	-1.832926
62	1	0	3.022720	2.595949	-2.175008
63	1	0	1.872673	1.329938	-2.689476
64	1	0	3.027055	0.994971	-1.391188
65	6	0	0.109012	2.407419	3.004587
66	1	0	-0.377849	2.397667	3.986835
67	1	0	0.717066	3.319547	2.995772
68	7	0	2.182273	-1.165788	-0.118580
69	7	0	1.742173	0.755020	1.779615
70	7	0	1.398886	2.240275	-0.833037
71	8	0	0.406754	-0.983025	-2.029127
72	8	0	1.598179	-2.326633	-3.408252
73	67	0	0.020951	0.033007	-0.020746

E(RTPSSh) = -1679.76667120

Zero-point correction= 0.619879 (Hartree/Particle)

Thermal correction to Energy= 0.653355

Thermal correction to Enthalpy= 0.654299

Thermal correction to Gibbs Free Energy= 0.559414

Sum of electronic and zero-point Energies= -1679.146792

Sum of electronic and thermal Energies= -1679.113316

Sum of electronic and thermal Enthalpies= -1679.112372

Sum of electronic and thermal Free Energies= -1679.207257

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.433644	-1.741352	-2.322513
2	6	0	2.461556	-1.866284	-1.212915
3	6	0	3.611617	-2.645530	-1.315481
4	1	0	3.805373	-3.193444	-2.230184
5	6	0	4.481825	-2.685477	-0.222318
6	1	0	5.392849	-3.273748	-0.268085
7	6	0	4.175788	-1.960861	0.932659
8	1	0	4.835862	-1.976626	1.793342
9	6	0	2.996865	-1.209173	0.962770
10	6	0	2.510253	-0.451700	2.174758
11	1	0	1.838249	-1.109145	2.733981
12	1	0	3.346746	-0.174043	2.830157
13	6	0	2.711893	1.767189	1.276907
14	1	0	3.505110	1.212782	0.767586
15	1	0	3.183012	2.291915	2.120003
16	6	0	2.123410	2.796447	0.323908
17	1	0	1.396965	3.420014	0.848136
18	1	0	2.932576	3.466678	-0.004155
19	6	0	-1.032230	2.638810	1.965748
20	1	0	-1.767727	3.326879	2.412127
21	1	0	-0.639246	3.154005	1.086810
22	6	0	0.996906	1.189907	3.018640
23	1	0	1.732186	1.350859	3.821768
24	1	0	0.402247	0.316816	3.299405
25	6	0	2.446555	1.746345	-1.852194
26	1	0	3.078492	2.584054	-2.182527
27	1	0	1.943559	1.312301	-2.717640
28	1	0	3.079640	0.980695	-1.401825
29	6	0	0.096488	2.439360	3.004190

30	1	0	-0.352639	2.438927	4.004447
31	1	0	0.712725	3.345120	2.969666
32	7	0	2.177095	-1.164515	-0.099952
33	7	0	1.728082	0.763459	1.783040
34	7	0	1.435967	2.211947	-0.869305
35	8	0	0.412532	-0.987370	-2.019923
36	8	0	1.612622	-2.332431	-3.390183
37	6	0	-1.201808	-2.406480	1.706575
38	6	0	-2.292655	-2.225086	0.667945
39	6	0	-3.437228	-3.016380	0.619981
40	1	0	-3.559311	-3.819685	1.336999
41	6	0	-4.399140	-2.730321	-0.353360
42	1	0	-5.309465	-3.318190	-0.415133
43	6	0	-4.186817	-1.675366	-1.243359
44	1	0	-4.921059	-1.427718	-2.002568
45	6	0	-3.001272	-0.937704	-1.143438
46	6	0	-2.623222	0.144079	-2.125035
47	1	0	-2.092056	-0.349546	-2.946618
48	1	0	-3.519447	0.615920	-2.550029
49	6	0	-2.451255	2.236449	-0.837378
50	1	0	-3.364284	2.518514	-1.381643
51	1	0	-1.828619	3.128856	-0.788125
52	6	0	-2.860152	1.804787	0.572821
53	1	0	-3.430993	2.629693	1.025586
54	1	0	-3.533346	0.946928	0.515692
55	6	0	0.662443	3.339776	-1.465758
56	1	0	1.363154	4.145359	-1.736748
57	1	0	0.038245	3.744122	-0.665505
58	6	0	-1.002686	1.737865	-2.807686
59	1	0	-1.749534	1.894869	-3.599207
60	1	0	-0.346212	0.927281	-3.136072
61	6	0	-2.364343	0.734938	2.649058
62	1	0	-3.070083	1.410777	3.154166
63	1	0	-1.605306	0.418544	3.362952
64	1	0	-2.907688	-0.145909	2.303682
65	6	0	-0.206498	3.046791	-2.695731

66	1	0	0.414367	3.072849	-3.598814
67	1	0	-0.885058	3.903321	-2.783676
68	7	0	-2.087032	-1.217276	-0.202741
69	7	0	-1.698226	1.191643	-1.588673
70	7	0	-1.737570	1.414739	1.486772
71	8	0	-0.242789	-1.529217	1.627638
72	8	0	-1.290081	-3.322766	2.528876
73	67	0	0.019621	0.041464	-0.017701

E(RTPSSh) = -1679.76686172

Zero-point correction= 0.619983 (Hartree/Particle)

Thermal correction to Energy= 0.653279

Thermal correction to Enthalpy= 0.654223

Thermal correction to Gibbs Free Energy= 0.560020

Sum of electronic and zero-point Energies= -1679.146879

Sum of electronic and thermal Energies= -1679.113583

Sum of electronic and thermal Enthalpies= -1679.112639

Sum of electronic and thermal Free Energies= -1679.206841

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.159883	-2.002789	2.229137
2	6	0	-2.243304	-2.107206	1.173466
3	6	0	-3.326183	-2.977695	1.266671
4	1	0	-3.414531	-3.628522	2.128633
5	6	0	-4.270679	-2.970111	0.235873
6	1	0	-5.133301	-3.627587	0.277616
7	6	0	-4.104374	-2.103237	-0.846851
8	1	0	-4.827791	-2.072777	-1.654608
9	6	0	-2.983654	-1.266870	-0.873756
10	6	0	-2.655783	-0.338687	-2.015988
11	1	0	-2.004815	-0.874871	-2.713228
12	1	0	-3.566959	-0.040616	-2.552406

13	6	0	-2.874807	1.730833	-0.808951
14	1	0	-3.491837	2.305768	-1.514075
15	1	0	-3.551184	1.058141	-0.273935
16	6	0	-2.240306	2.698661	0.182520
17	1	0	-1.665146	3.452782	-0.353015
18	1	0	-3.048163	3.235017	0.702318
19	6	0	0.521884	3.159147	-1.778702
20	1	0	1.201610	3.872437	-2.270256
21	1	0	0.090273	3.695702	-0.934658
22	6	0	-1.336969	1.469912	-2.801605
23	1	0	-2.153250	1.587038	-3.530751
24	1	0	-0.668098	0.697419	-3.188949
25	6	0	-2.167251	1.451462	2.265432
26	1	0	-2.789126	2.221660	2.744643
27	1	0	-1.525799	0.988369	3.015528
28	1	0	-2.817052	0.682016	1.845007
29	6	0	-0.599607	2.819351	-2.783907
30	1	0	-0.195920	2.894722	-3.800342
31	1	0	-1.327059	3.635890	-2.703081
32	7	0	-2.085944	-1.277520	0.124482
33	7	0	-1.905352	0.869947	-1.550067
34	7	0	-1.335023	2.055939	1.190536
35	8	0	-0.236689	-1.124658	1.954318
36	8	0	-1.215208	-2.714398	3.235698
37	6	0	1.157818	-2.005364	-2.227654
38	6	0	2.241595	-2.109458	-1.172311
39	6	0	3.324450	-2.979969	-1.265621
40	1	0	3.412416	-3.631186	-2.127326
41	6	0	4.269475	-2.971842	-0.235314
42	1	0	5.132118	-3.629283	-0.277201
43	6	0	4.103683	-2.104451	0.847081
44	1	0	4.827504	-2.073572	1.654458
45	6	0	2.982902	-1.268177	0.874190
46	6	0	2.655526	-0.339429	2.016084
47	1	0	2.003966	-0.874838	2.713361
48	1	0	3.566810	-0.041875	2.552583

49	6	0	2.876230	1.729377	0.807995
50	1	0	3.552333	1.055970	0.273517
51	1	0	3.493435	2.304429	1.512805
52	6	0	2.242376	2.696930	-0.184207
53	1	0	1.667910	3.451957	0.350824
54	1	0	3.050603	3.232232	-0.704512
55	6	0	-0.519407	3.160609	1.776721
56	1	0	-1.198435	3.875041	2.267588
57	1	0	-0.087130	3.695979	0.932274
58	6	0	1.338111	1.470646	2.800757
59	1	0	2.154467	1.587656	3.529833
60	1	0	0.668768	0.698767	3.188511
61	6	0	2.168132	1.448037	-2.266020
62	1	0	2.790652	2.217286	-2.745911
63	1	0	1.526280	0.984825	-3.015681
64	1	0	2.817296	0.678441	-1.844891
65	6	0	0.601569	2.820523	2.782363
66	1	0	0.197668	2.896548	3.798667
67	1	0	1.329522	3.636604	2.701390
68	7	0	2.084694	-1.279329	-0.123611
69	7	0	1.906122	0.869627	1.549536
70	7	0	1.336436	2.054184	-1.191607
71	8	0	0.235159	-1.126550	-1.953249
72	8	0	1.212435	-2.717862	-3.233631
73	67	0	0.000009	0.053866	0.000162

E(RTPSSh) = -1679.76040936

Zero-point correction= 0.619331 (Hartree/Particle)

Thermal correction to Energy= 0.653105

Thermal correction to Enthalpy= 0.654049

Thermal correction to Gibbs Free Energy= 0.558514

Sum of electronic and zero-point Energies= -1679.141078

Sum of electronic and thermal Energies= -1679.107304

Sum of electronic and thermal Enthalpies= -1679.106360

Sum of electronic and thermal Free Energies= -1679.201895

[Yb(Me$_2$tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.340934	-2.150523	1.883170
2	6	0	-2.384186	-2.041206	0.786863
3	6	0	-3.546571	-2.806565	0.755513
4	1	0	-3.728154	-3.533369	1.538549
5	6	0	-4.448104	-2.595870	-0.292353
6	1	0	-5.370021	-3.166216	-0.346004
7	6	0	-4.159529	-1.641441	-1.270386
8	1	0	-4.844845	-1.457370	-2.090966
9	6	0	-2.962278	-0.921628	-1.176696
10	6	0	-2.501163	0.050321	-2.236650
11	1	0	-1.963743	-0.536670	-2.989193
12	1	0	-3.358413	0.520239	-2.737176
13	6	0	-2.289163	2.251396	-1.160332
14	1	0	-3.119841	2.549713	-1.816426
15	1	0	-1.604651	3.100223	-1.111260
16	6	0	-2.846070	1.954280	0.227869
17	1	0	-3.422337	2.830501	0.562111
18	1	0	-3.544315	1.115857	0.181354
19	6	0	1.116242	2.869410	-1.668429
20	1	0	1.871053	3.624790	-1.938540
21	1	0	0.589226	3.263370	-0.795165
22	6	0	-0.782550	1.524996	-2.971435
23	1	0	-1.493763	1.742401	-3.781903
24	1	0	-0.212833	0.640586	-3.268582
25	6	0	-2.529768	1.048740	2.415664
26	1	0	-3.217121	1.793247	2.844208
27	1	0	-1.826729	0.728999	3.183489
28	1	0	-3.109779	0.182283	2.094934

29	6	0	0.147454	2.741953	-2.855959
30	1	0	0.722585	2.742450	-3.789242
31	1	0	-0.437272	3.668564	-2.877316
32	7	0	-2.110323	-1.125010	-0.162065
33	7	0	-1.549956	1.100839	-1.753240
34	7	0	-1.806308	1.614636	1.248360
35	8	0	-0.337986	-1.330133	1.743023
36	8	0	-1.497866	-2.963625	2.797976
37	6	0	1.341019	-2.150260	-1.883454
38	6	0	2.384229	-2.041107	-0.787092
39	6	0	3.546592	-2.806501	-0.755790
40	1	0	3.728175	-3.533233	-1.538892
41	6	0	4.448107	-2.595934	0.292118
42	1	0	5.370005	-3.166314	0.345740
43	6	0	4.159539	-1.641588	1.270234
44	1	0	4.844835	-1.457620	2.090852
45	6	0	2.962305	-0.921741	1.176591
46	6	0	2.501189	0.050100	2.236642
47	1	0	1.963763	-0.536967	2.989123
48	1	0	3.358435	0.519967	2.737221
49	6	0	2.289170	2.251301	1.160582
50	1	0	3.119861	2.549534	1.816699
51	1	0	1.604652	3.100130	1.111642
52	6	0	2.846044	1.954401	-0.227678
53	1	0	3.422290	2.830677	-0.561807
54	1	0	3.544300	1.115979	-0.181309
55	6	0	-1.116357	2.869094	1.668836
56	1	0	-1.871202	3.624398	1.939063
57	1	0	-0.589356	3.263220	0.795640
58	6	0	0.782567	1.524620	2.971614
59	1	0	1.493786	1.741975	3.782089
60	1	0	0.212935	0.640124	3.268668
61	6	0	2.529650	1.049227	-2.415630
62	1	0	3.216974	1.793817	-2.844077
63	1	0	1.826563	0.729626	-3.183470
64	1	0	3.109684	0.182712	-2.095097

65	6	0	-0.147541	2.741516	2.856333
66	1	0	-0.722656	2.741837	3.789626
67	1	0	0.437118	3.668166	2.877821
68	7	0	2.110363	-1.125003	0.161925
69	7	0	1.549974	1.100660	1.753350
70	7	0	1.806248	1.614902	-1.248184
71	8	0	0.338044	-1.329919	-1.743202
72	8	0	1.497891	-2.963359	-2.798273
73	70	0	0.000011	0.048708	-0.000007

E(RTPSSh) = -1681.52118252

Zero-point correction= 0.621403 (Hartree/Particle)

Thermal correction to Energy= 0.654149

Thermal correction to Enthalpy= 0.655093

Thermal correction to Gibbs Free Energy= 0.562289

Sum of electronic and zero-point Energies= -1680.899779

Sum of electronic and thermal Energies= -1680.867033

Sum of electronic and thermal Enthalpies= -1680.866089

Sum of electronic and thermal Free Energies= -1680.958894

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.149608	-2.384994	1.715142
2	6	0	-2.252023	-2.214670	0.689562
3	6	0	-3.394528	-3.009171	0.654983
4	1	0	-3.508515	-3.809522	1.376654
5	6	0	-4.365031	-2.729376	-0.311490
6	1	0	-5.274494	-3.319482	-0.363387
7	6	0	-4.162229	-1.677201	-1.207055
8	1	0	-4.903295	-1.433993	-1.961005
9	6	0	-2.978476	-0.935251	-1.118878
10	6	0	-2.610301	0.147816	-2.101060
11	1	0	-2.073381	-0.341176	-2.921301

12	1	0	-3.509735	0.614234	-2.524982
13	6	0	-2.456279	2.230046	-0.798128
14	1	0	-3.380302	2.498626	-1.330230
15	1	0	-1.848801	3.133336	-0.749962
16	6	0	-2.836075	1.780877	0.612456
17	1	0	-3.395313	2.599698	1.089899
18	1	0	-3.509083	0.922731	0.560521
19	6	0	0.633477	3.369074	-1.426467
20	1	0	1.352140	4.157548	-1.699733
21	1	0	0.021007	3.790297	-0.625686
22	6	0	-1.023687	1.772410	-2.781013
23	1	0	-1.784667	1.934007	-3.558142
24	1	0	-0.364528	0.974430	-3.132340
25	6	0	-2.296860	0.720974	2.678062
26	1	0	-2.966451	1.416274	3.204794
27	1	0	-1.525207	0.379950	3.365812
28	1	0	-2.876451	-0.143321	2.349886
29	6	0	-0.241584	3.088371	-2.655849
30	1	0	0.374299	3.133770	-3.561412
31	1	0	-0.929467	3.938659	-2.728187
32	7	0	-2.055594	-1.208744	-0.185133
33	7	0	-1.693421	1.200777	-1.561183
34	7	0	-1.690952	1.380680	1.492838
35	8	0	-0.198083	-1.501605	1.614376
36	8	0	-1.219733	-3.294420	2.546271
37	6	0	1.342755	-1.709802	-2.345712
38	6	0	2.393230	-1.861789	-1.263476
39	6	0	3.526514	-2.660077	-1.395937
40	1	0	3.691255	-3.204937	-2.318099
41	6	0	4.418650	-2.723471	-0.321495
42	1	0	5.317958	-3.327311	-0.390031
43	6	0	4.148363	-2.002157	0.844087
44	1	0	4.825069	-2.035525	1.691294
45	6	0	2.983357	-1.230467	0.903778
46	6	0	2.535330	-0.476251	2.130868
47	1	0	1.877830	-1.133133	2.707061

48	1	0	3.391132	-0.202244	2.762280
49	6	0	2.727579	1.747129	1.254702
50	1	0	3.505635	1.194665	0.720461
51	1	0	3.220363	2.253625	2.096565
52	6	0	2.129890	2.795018	0.329133
53	1	0	1.442667	3.440238	0.878477
54	1	0	2.943502	3.442174	-0.031964
55	6	0	-0.942385	2.595446	1.927112
56	1	0	-1.652392	3.347945	2.304525
57	1	0	-0.487204	3.025409	1.032809
58	6	0	1.046573	1.159597	3.018603
59	1	0	1.798524	1.322776	3.805564
60	1	0	0.461362	0.283778	3.309248
61	6	0	2.367332	1.740710	-1.846619
62	1	0	3.000101	2.570857	-2.193135
63	1	0	1.838014	1.312185	-2.698388
64	1	0	3.003028	0.968822	-1.411740
65	6	0	0.141054	2.402044	3.006682
66	1	0	-0.339692	2.394732	3.991924
67	1	0	0.751227	3.312661	2.992302
68	7	0	2.142578	-1.162288	-0.140703
69	7	0	1.746677	0.741972	1.763744
70	7	0	1.387195	2.223705	-0.836646
71	8	0	0.343742	-0.941184	-2.007117
72	8	0	1.481826	-2.291681	-3.424006
73	70	0	0.018375	0.042523	-0.010842

E(RTPSSh) = -1681.51404763

Zero-point correction= 0.620363 (Hartree/Particle)

Thermal correction to Energy= 0.653692

Thermal correction to Enthalpy= 0.654636

Thermal correction to Gibbs Free Energy= 0.560238

Sum of electronic and zero-point Energies= -1680.893685

Sum of electronic and thermal Energies= -1680.860356

Sum of electronic and thermal Enthalpies= -1680.859411

Sum of electronic and thermal Free Energies= -1680.953809

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.350558	-1.722074	-2.325246
2	6	0	2.393924	-1.869450	-1.235521
3	6	0	3.527972	-2.668600	-1.356507
4	1	0	3.699726	-3.216447	-2.275644
5	6	0	4.411299	-2.728866	-0.274735
6	1	0	5.310901	-3.333258	-0.334137
7	6	0	4.131914	-2.003869	0.886536
8	1	0	4.801664	-2.035218	1.739306
9	6	0	2.967391	-1.230701	0.934107
10	6	0	2.509993	-0.468690	2.153187
11	1	0	1.844063	-1.119302	2.726513
12	1	0	3.360457	-0.193645	2.791436
13	6	0	2.723057	1.743613	1.257440
14	1	0	3.507239	1.181254	0.742938
15	1	0	3.204429	2.262844	2.098021
16	6	0	2.137577	2.775421	0.308357
17	1	0	1.421632	3.407460	0.836965
18	1	0	2.949144	3.437015	-0.030778
19	6	0	-1.002569	2.634214	1.966639
20	1	0	-1.738738	3.322588	2.411035
21	1	0	-0.608962	3.146591	1.086448
22	6	0	1.020844	1.183371	3.013522
23	1	0	1.768265	1.343207	3.805555
24	1	0	0.426526	0.313615	3.303747
25	6	0	2.433786	1.719322	-1.867404
26	1	0	3.066016	2.554308	-2.203780
27	1	0	1.920484	1.287489	-2.727642
28	1	0	3.067631	0.951582	-1.422128
29	6	0	0.125906	2.435683	3.004049
30	1	0	-0.320898	2.438085	4.005317
31	1	0	0.744786	3.339526	2.966013

32	7	0	2.135446	-1.165355	-0.117636
33	7	0	1.731010	0.750523	1.768563
34	7	0	1.434334	2.190988	-0.875687
35	8	0	0.348614	-0.953891	-1.995558
36	8	0	1.497561	-2.307560	-3.400713
37	6	0	-1.156525	-2.377481	1.716865
38	6	0	-2.253343	-2.213711	0.684439
39	6	0	-3.389314	-3.016836	0.640247
40	1	0	-3.501590	-3.820416	1.358580
41	6	0	-4.356175	-2.741371	-0.331293
42	1	0	-5.260874	-3.338081	-0.390603
43	6	0	-4.155371	-1.685485	-1.222618
44	1	0	-4.893089	-1.445618	-1.980946
45	6	0	-2.976953	-0.935898	-1.125561
46	6	0	-2.609314	0.147220	-2.107299
47	1	0	-2.081112	-0.344594	-2.931447
48	1	0	-3.508783	0.618426	-2.525928
49	6	0	-2.438763	2.238535	-0.822791
50	1	0	-3.354460	2.516171	-1.364647
51	1	0	-1.819950	3.133764	-0.774919
52	6	0	-2.839052	1.802128	0.587293
53	1	0	-3.405810	2.624546	1.049173
54	1	0	-3.512062	0.944077	0.531855
55	6	0	0.669692	3.329254	-1.465528
56	1	0	1.378815	4.128408	-1.733317
57	1	0	0.051447	3.735954	-0.661967
58	6	0	-1.004654	1.744442	-2.801203
59	1	0	-1.763532	1.905200	-3.580472
60	1	0	-0.354753	0.933570	-3.140216
61	6	0	-2.327307	0.727072	2.655217
62	1	0	-3.027301	1.404220	3.166170
63	1	0	-1.564402	0.406279	3.362604
64	1	0	-2.876099	-0.150892	2.311413
65	6	0	-0.204497	3.049811	-2.693303
66	1	0	0.412248	3.077060	-3.599124
67	1	0	-0.879649	3.909780	-2.773673

68	7	0	-2.058382	-1.204018	-0.186473
69	7	0	-1.682816	1.195560	-1.573952
70	7	0	-1.707627	1.408798	1.489508
71	8	0	-0.212402	-1.485632	1.624592
72	8	0	-1.224564	-3.289625	2.545342
73	70	0	0.016553	0.050433	-0.009066

E(RTPSSh) = -1681.51420424

Zero-point correction= 0.620562 (Hartree/Particle)

Thermal correction to Energy= 0.653658

Thermal correction to Enthalpy= 0.654602

Thermal correction to Gibbs Free Energy= 0.561049

Sum of electronic and zero-point Energies= -1680.893642

Sum of electronic and thermal Energies= -1680.860546

Sum of electronic and thermal Enthalpies= -1680.859602

Sum of electronic and thermal Free Energies= -1680.953155

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.067965	-1.981364	2.235240
2	6	0	-2.169346	-2.108730	1.204037
3	6	0	-3.233248	-2.999297	1.317097
4	1	0	-3.293166	-3.652369	2.179818
5	6	0	-4.197167	-3.008619	0.304334
6	1	0	-5.046331	-3.682293	0.361076
7	6	0	-4.066959	-2.136921	-0.779240
8	1	0	-4.805594	-2.117919	-1.573526
9	6	0	-2.962488	-1.279675	-0.825647
10	6	0	-2.674810	-0.342548	-1.969303
11	1	0	-2.042042	-0.869374	-2.689284
12	1	0	-3.602914	-0.044043	-2.475404
13	6	0	-2.880261	1.717947	-0.752705
14	1	0	-3.514255	2.290690	-1.444503

15	1	0	-3.542245	1.040067	-0.206223
16	6	0	-2.230000	2.685224	0.226768
17	1	0	-1.670588	3.443964	-0.318762
18	1	0	-3.027335	3.215686	0.768093
19	6	0	0.485530	3.153358	-1.785711
20	1	0	1.165068	3.859448	-2.287407
21	1	0	0.073395	3.693907	-0.934667
22	6	0	-1.388509	1.473684	-2.777649
23	1	0	-2.225983	1.591281	-3.482255
24	1	0	-0.728218	0.705640	-3.186861
25	6	0	-2.108818	1.435757	2.303664
26	1	0	-2.720846	2.206347	2.794512
27	1	0	-1.451963	0.972986	3.039971
28	1	0	-2.767134	0.666478	1.896578
29	6	0	-0.655946	2.824115	-2.770124
30	1	0	-0.274404	2.908030	-3.794362
31	1	0	-1.382909	3.638555	-2.666972
32	7	0	-2.045306	-1.274184	0.154283
33	7	0	-1.918408	0.865872	-1.513509
34	7	0	-1.298916	2.041699	1.211540
35	8	0	-0.171217	-1.084858	1.934411
36	8	0	-1.083656	-2.688956	3.245891
37	6	0	1.065619	-1.983991	-2.233825
38	6	0	2.167362	-2.111176	-1.202991
39	6	0	3.230965	-3.002094	-1.316074
40	1	0	3.290318	-3.655595	-2.178506
41	6	0	4.195344	-3.011180	-0.303747
42	1	0	5.044307	-3.685098	-0.360562
43	6	0	4.065843	-2.138938	0.779478
44	1	0	4.804801	-2.119789	1.573457
45	6	0	2.961610	-1.281393	0.825976
46	6	0	2.674595	-0.343680	1.969317
47	1	0	2.041232	-0.869690	2.689369
48	1	0	3.602866	-0.045805	2.475457
49	6	0	2.881897	1.716158	0.751804
50	1	0	3.543566	1.037566	0.205810

51	1	0	3.516152	2.288907	1.443339
52	6	0	2.232445	2.683341	-0.228351
53	1	0	1.673911	3.443086	0.316687
54	1	0	3.030261	3.212549	-0.770193
55	6	0	-0.482606	3.154632	1.783708
56	1	0	-1.161339	3.862096	2.284570
57	1	0	-0.069650	3.693769	0.932183
58	6	0	1.389950	1.474097	2.776853
59	1	0	2.227581	1.591481	3.481309
60	1	0	0.729191	0.706691	3.186498
61	6	0	2.109905	1.432187	-2.304046
62	1	0	2.722985	2.201625	-2.795377
63	1	0	1.452616	0.969672	-3.040111
64	1	0	2.767187	0.662433	-1.896191
65	6	0	0.658209	2.824977	2.768698
66	1	0	0.276307	2.909425	3.792759
67	1	0	1.385658	3.638990	2.665557
68	7	0	2.044023	-1.276070	-0.153591
69	7	0	1.919312	0.865248	1.512971
70	7	0	1.300569	2.040007	-1.212500
71	8	0	0.169367	-1.086916	-1.933257
72	8	0	1.080575	-2.692348	-3.243961
73	70	0	0.000045	0.068600	0.000139

E(RTPSSh) = -1681.50742736

Zero-point correction= 0.619672 (Hartree/Particle)

Thermal correction to Energy= 0.653355

Thermal correction to Enthalpy= 0.654299

Thermal correction to Gibbs Free Energy= 0.559030

Sum of electronic and zero-point Energies= -1680.887755

Sum of electronic and thermal Energies= -1680.854072

Sum of electronic and thermal Enthalpies= -1680.853128

Sum of electronic and thermal Free Energies= -1680.948398

[Lu(Me_2tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.337530	-2.154401	-1.877918
2	6	0	2.382322	-2.039688	-0.784251
3	6	0	3.546924	-2.801092	-0.751320
4	1	0	3.729881	-3.530782	-1.531319
5	6	0	4.449349	-2.582392	0.294332
6	1	0	5.373229	-3.149384	0.349197
7	6	0	4.159193	-1.624464	1.268302
8	1	0	4.845162	-1.434314	2.086910
9	6	0	2.959240	-0.909083	1.173566
10	6	0	2.496564	0.064472	2.230797
11	1	0	1.968051	-0.523701	2.988687
12	1	0	3.353003	0.542564	2.724763
13	6	0	2.263816	2.266323	1.160013
14	1	0	3.086736	2.574684	1.821222
15	1	0	1.570200	3.107264	1.104846
16	6	0	2.830318	1.968849	-0.222384
17	1	0	3.405238	2.845285	-0.557799
18	1	0	3.531251	1.133042	-0.169886
19	6	0	-1.121182	2.878405	1.686587
20	1	0	-1.887944	3.616669	1.970332
21	1	0	-0.601060	3.300876	0.822815
22	6	0	0.774176	1.523489	2.976066
23	1	0	1.491027	1.734568	3.783196
24	1	0	0.205889	0.637583	3.271063
25	6	0	2.523004	1.043117	-2.401609
26	1	0	3.215828	1.782055	-2.830875
27	1	0	1.824232	0.720550	-3.171910
28	1	0	3.098104	0.177535	-2.070553
29	6	0	-0.153417	2.742027	2.873285
30	1	0	-0.729001	2.734298	3.806214

31	1	0	0.432448	3.667596	2.903247
32	71	0	0.000000	0.027367	-0.000006
33	7	0	2.106707	-1.119985	0.161177
34	7	0	1.533953	1.107629	1.750690
35	7	0	1.793768	1.623000	-1.243596
36	8	0	0.332971	-1.335049	-1.736079
37	8	0	1.492102	-2.969269	-2.790844
38	6	0	-1.337144	-2.154952	1.877496
39	6	0	-2.382199	-2.039874	0.784117
40	6	0	-3.546825	-2.801244	0.751221
41	1	0	-3.729691	-3.531064	1.531120
42	6	0	-4.449345	-2.582408	-0.294321
43	1	0	-5.373233	-3.149390	-0.349171
44	6	0	-4.159241	-1.624410	-1.268238
45	1	0	-4.845263	-1.434185	-2.086783
46	6	0	-2.959268	-0.909059	-1.173534
47	6	0	-2.496622	0.064522	-2.230756
48	1	0	-1.968148	-0.523631	-2.988689
49	1	0	-3.353078	0.542640	-2.724671
50	6	0	-2.263835	2.266342	-1.159959
51	1	0	-3.086753	2.574724	-1.821160
52	1	0	-1.570214	3.107279	-1.104767
53	6	0	-2.830343	1.968828	0.222426
54	1	0	-3.405268	2.845254	0.557859
55	1	0	-3.531269	1.133017	0.169906
56	6	0	1.121158	2.878433	-1.686562
57	1	0	1.887920	3.616694	-1.970313
58	1	0	0.601039	3.300917	-0.822794
59	6	0	-0.774217	1.523526	-2.976043
60	1	0	-1.491074	1.734620	-3.783162
61	1	0	-0.205944	0.637619	-3.271057
62	6	0	-2.523004	1.043083	2.401648
63	1	0	-3.215818	1.782021	2.830929
64	1	0	-1.824219	0.720513	3.171935
65	1	0	-3.098115	0.177506	2.070599
66	6	0	0.153389	2.742056	-2.873261

67	1	0	0.728972	2.734321	-3.806190
68	1	0	-0.432468	3.667629	-2.903226
69	7	0	-2.106679	-1.120037	-0.161209
70	7	0	-1.533984	1.107656	-1.750663
71	7	0	-1.793787	1.622969	1.243625
72	8	0	-0.332962	-1.335076	1.736040
73	8	0	-1.492296	-2.968979	2.791075

E(RTPSSh) = -1682.07371355

Zero-point correction= 0.621780 (Hartree/Particle)

Thermal correction to Energy= 0.654498

Thermal correction to Enthalpy= 0.655442

Thermal correction to Gibbs Free Energy= 0.562600

Sum of electronic and zero-point Energies= -1681.451934

Sum of electronic and thermal Energies= -1681.419215

Sum of electronic and thermal Enthalpies= -1681.418271

Sum of electronic and thermal Free Energies= -1681.511114

F2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.125967	-2.400663	1.695292
2	6	0	-2.237129	-2.220480	0.681856
3	6	0	-3.380593	-3.013453	0.647452
4	1	0	-3.490969	-3.820461	1.362271
5	6	0	-4.356755	-2.723521	-0.310372
6	1	0	-5.267416	-3.311833	-0.361852
7	6	0	-4.157720	-1.663963	-1.198037
8	1	0	-4.902779	-1.413328	-1.945607
9	6	0	-2.972746	-0.923892	-1.110024
10	6	0	-2.607369	0.166647	-2.084154
11	1	0	-2.073999	-0.316460	-2.909992
12	1	0	-3.507530	0.638408	-2.500448
13	6	0	-2.447392	2.236572	-0.767383

14	1	0	-3.370292	2.512937	-1.297604
15	1	0	-1.839251	3.138606	-0.707499
16	6	0	-2.826941	1.768214	0.635179
17	1	0	-3.385725	2.578787	1.126823
18	1	0	-3.497774	0.909144	0.573782
19	6	0	0.628263	3.386011	-1.404842
20	1	0	1.354239	4.167895	-1.677498
21	1	0	0.023679	3.810769	-0.599862
22	6	0	-1.029988	1.797778	-2.760811
23	1	0	-1.799236	1.961710	-3.529254
24	1	0	-0.370987	1.005367	-3.123993
25	6	0	-2.270857	0.694835	2.688652
26	1	0	-2.933040	1.388550	3.226489
27	1	0	-1.494141	0.345979	3.366540
28	1	0	-2.856480	-0.164999	2.359504
29	6	0	-0.254116	3.116235	-2.631141
30	1	0	0.355325	3.172584	-3.540390
31	1	0	-0.946436	3.963856	-2.690818
32	7	0	-2.045164	-1.205962	-0.183730
33	7	0	-1.686179	1.214396	-1.539320
34	7	0	-1.674724	1.361329	1.501800
35	8	0	-0.173232	-1.518924	1.588426
36	8	0	-1.188494	-3.314854	2.521468
37	6	0	1.310010	-1.683184	-2.358525
38	6	0	2.367174	-1.853970	-1.286660
39	6	0	3.491570	-2.662124	-1.432361
40	1	0	3.645021	-3.202379	-2.359204
41	6	0	4.390126	-2.741386	-0.364208
42	1	0	5.282930	-3.353638	-0.442693
43	6	0	4.134541	-2.024863	0.807607
44	1	0	4.816692	-2.069829	1.649943
45	6	0	2.977273	-1.242493	0.880080
46	6	0	2.544623	-0.491183	2.114228
47	1	0	1.892677	-1.148483	2.696036
48	1	0	3.407970	-0.220131	2.736627
49	6	0	2.734220	1.734875	1.247391

50	1	0	3.505691	1.184428	0.701657
51	1	0	3.236461	2.232655	2.088835
52	6	0	2.130833	2.791555	0.336712
53	1	0	1.452379	3.436063	0.897507
54	1	0	2.943025	3.437430	-0.029884
55	6	0	-0.927821	2.577493	1.932197
56	1	0	-1.638536	3.327444	2.313369
57	1	0	-0.485061	3.006779	1.031656
58	6	0	1.065678	1.145808	3.017670
59	1	0	1.823584	1.310628	3.798563
60	1	0	0.483719	0.269914	3.314516
61	6	0	2.343841	1.747391	-1.844238
62	1	0	2.979860	2.576084	-2.188257
63	1	0	1.806445	1.329195	-2.695832
64	1	0	2.977328	0.967986	-1.419824
65	6	0	0.159408	2.387512	3.008161
66	1	0	-0.319500	2.380656	3.994308
67	1	0	0.768532	3.298703	2.992087
68	7	0	2.130019	-1.159650	-0.157827
69	7	0	1.754753	0.729076	1.757375
70	7	0	1.373153	2.230136	-0.824103
71	8	0	0.320868	-0.909464	-2.002593
72	8	0	1.433870	-2.254847	-3.444017
73	71	0	0.017232	0.042731	-0.003295

E(RTPSSh) = -1682.06829660

Zero-point correction= 0.620427 (Hartree/Particle)

Thermal correction to Energy= 0.653678

Thermal correction to Enthalpy= 0.654622

Thermal correction to Gibbs Free Energy= 0.560518

Sum of electronic and zero-point Energies= -1681.447870

Sum of electronic and thermal Energies= -1681.414619

Sum of electronic and thermal Enthalpies= -1681.413675

Sum of electronic and thermal Free Energies= -1681.507779

F3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.310389	-1.682267	-2.358821
2	6	0	2.367447	-1.853462	-1.286911
3	6	0	3.492264	-2.660973	-1.433062
4	1	0	3.646009	-3.200496	-2.360261
5	6	0	4.390773	-2.740466	-0.364919
6	1	0	5.283919	-3.352143	-0.443731
7	6	0	4.134732	-2.024833	0.807362
8	1	0	4.816830	-2.070033	1.649706
9	6	0	2.977096	-1.243086	0.880256
10	6	0	2.544087	-0.492383	2.114667
11	1	0	1.891971	-1.149784	2.696082
12	1	0	3.407200	-0.221273	2.737293
13	6	0	2.733910	1.734053	1.249122
14	1	0	3.505409	1.183941	0.703119
15	1	0	3.235693	2.231013	2.091281
16	6	0	2.130694	2.791292	0.338818
17	1	0	1.451788	3.435303	0.899644
18	1	0	2.942901	3.437536	-0.026992
19	6	0	-0.928780	2.576058	1.931813
20	1	0	-1.639216	3.326526	2.312507
21	1	0	-0.485247	3.004953	1.031448
22	6	0	1.064002	1.143934	3.018043
23	1	0	1.821209	1.308375	3.799656
24	1	0	0.481920	0.267771	3.313783
25	6	0	2.344723	1.748095	-1.842661
26	1	0	2.980658	2.577033	-2.186169
27	1	0	1.807583	1.330105	-2.694478
28	1	0	2.978172	0.968658	-1.418366
29	6	0	0.157730	2.385573	3.008418
30	1	0	-0.321813	2.378418	3.994238
31	1	0	0.766841	3.296779	2.993060

32	7	0	2.129858	-1.160043	-0.157643
33	7	0	1.754165	0.728003	1.757995
34	7	0	1.373591	2.230345	-0.822610
35	8	0	0.321852	-0.907710	-2.003094
36	8	0	1.433949	-2.254112	-3.444242
37	6	0	-1.126667	-2.400378	1.695393
38	6	0	-2.237100	-2.220533	0.681072
39	6	0	-3.380416	-3.013685	0.645812
40	1	0	-3.491201	-3.820655	1.360580
41	6	0	-4.355871	-2.723948	-0.312792
42	1	0	-5.266354	-3.312441	-0.365020
43	6	0	-4.156369	-1.664299	-1.200246
44	1	0	-4.900885	-1.413792	-1.948377
45	6	0	-2.971614	-0.923979	-1.111294
46	6	0	-2.606059	0.166910	-2.084967
47	1	0	-2.072200	-0.315732	-2.910734
48	1	0	-3.506213	0.638460	-2.501521
49	6	0	-2.447662	2.236575	-0.767730
50	1	0	-3.370148	2.512858	-1.298705
51	1	0	-1.839794	3.138719	-0.707038
52	6	0	-2.828068	1.767637	0.634385
53	1	0	-3.386989	2.578000	1.126154
54	1	0	-3.498890	0.908612	0.572253
55	6	0	0.629017	3.386534	-1.403189
56	1	0	1.355223	4.168384	-1.675325
57	1	0	0.024261	3.811151	-0.598248
58	6	0	-1.029054	1.798949	-2.760383
59	1	0	-1.798163	1.963399	-3.528857
60	1	0	-0.370055	1.006732	-3.123930
61	6	0	-2.272524	0.694049	2.688076
62	1	0	-2.934495	1.387981	3.225859
63	1	0	-1.495818	0.345094	3.365926
64	1	0	-2.858399	-0.165632	2.359036
65	6	0	-0.253084	3.117334	-2.629822
66	1	0	0.356528	3.174074	-3.538923
67	1	0	-0.945358	3.964984	-2.689270

68	7	0	-2.044675	-1.206006	-0.184353
69	7	0	-1.685496	1.214833	-1.539395
70	7	0	-1.676211	1.360245	1.501172
71	8	0	-0.173886	-1.518663	1.589059
72	8	0	-1.189942	-3.314245	2.521893
73	71	0	0.017340	0.042917	-0.003231

E(RTPSSh) = -1682.06829532

Zero-point correction= 0.620433 (Hartree/Particle)

Thermal correction to Energy= 0.653682

Thermal correction to Enthalpy= 0.654627

Thermal correction to Gibbs Free Energy= 0.560528

Sum of electronic and zero-point Energies= -1681.447863

Sum of electronic and thermal Energies= -1681.414613

Sum of electronic and thermal Enthalpies= -1681.413669

Sum of electronic and thermal Free Energies= -1681.507767

F4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.032820	-1.985535	2.229569
2	6	0	-2.146999	-2.110371	1.213615
3	6	0	-3.206811	-3.004538	1.334592
4	1	0	-3.256056	-3.660460	2.195835
5	6	0	-4.179863	-3.014677	0.330677
6	1	0	-5.026125	-3.691498	0.392940
7	6	0	-4.061169	-2.140304	-0.751934
8	1	0	-4.805757	-2.122464	-1.540701
9	6	0	-2.960191	-1.278884	-0.805598
10	6	0	-2.684941	-0.340900	-1.950803
11	1	0	-2.060393	-0.867440	-2.677809
12	1	0	-3.618017	-0.040745	-2.446572
13	6	0	-2.882363	1.718615	-0.735892
14	1	0	-3.518421	2.292449	-1.424817

15	1	0	-3.542979	1.040765	-0.187728
16	6	0	-2.227261	2.683380	0.241905
17	1	0	-1.672213	3.444536	-0.304695
18	1	0	-3.021097	3.211144	0.790810
19	6	0	0.473431	3.150811	-1.789086
20	1	0	1.152457	3.855303	-2.293526
21	1	0	0.065926	3.692159	-0.936378
22	6	0	-1.403264	1.472081	-2.769544
23	1	0	-2.245474	1.587078	-3.468829
24	1	0	-0.744946	0.703832	-3.181612
25	6	0	-2.091946	1.428649	2.314527
26	1	0	-2.695544	2.199572	2.815026
27	1	0	-1.430851	0.958703	3.042459
28	1	0	-2.758320	0.665334	1.909326
29	6	0	-0.672444	2.822794	-2.767987
30	1	0	-0.296231	2.906793	-3.794171
31	1	0	-1.399311	3.636785	-2.660856
32	7	0	-2.034557	-1.271059	0.166396
33	7	0	-1.923695	0.866318	-1.500533
34	7	0	-1.288792	2.037015	1.218276
35	8	0	-0.137152	-1.093873	1.911763
36	8	0	-1.035205	-2.690191	3.242207
37	6	0	1.031480	-1.987181	-2.228590
38	6	0	2.145912	-2.111822	-1.212897
39	6	0	3.205716	-3.005982	-1.333989
40	1	0	3.254679	-3.662143	-2.195064
41	6	0	4.179164	-3.015747	-0.330454
42	1	0	5.025465	-3.692504	-0.392861
43	6	0	4.060833	-2.141055	0.751942
44	1	0	4.805718	-2.122931	1.540421
45	6	0	2.959798	-1.279722	0.805793
46	6	0	2.684914	-0.341379	1.950791
47	1	0	2.060173	-0.867471	2.677955
48	1	0	3.618102	-0.041415	2.446451
49	6	0	2.883130	1.717773	0.735343
50	1	0	3.543676	1.039570	0.187520

51	1	0	3.519281	2.291720	1.424106
52	6	0	2.228438	2.682412	-0.242891
53	1	0	1.673869	3.444154	0.303393
54	1	0	3.022536	3.209455	-0.792108
55	6	0	-0.471953	3.151490	1.787806
56	1	0	-1.150506	3.856827	2.291718
57	1	0	-0.063946	3.691962	0.934791
58	6	0	1.403916	1.472346	2.769045
59	1	0	2.246186	1.587257	3.468275
60	1	0	0.745346	0.704433	3.181330
61	6	0	2.092404	1.426613	-2.314749
62	1	0	2.696650	2.196851	-2.815510
63	1	0	1.431084	0.956808	-3.042555
64	1	0	2.758145	0.663025	-1.909035
65	6	0	0.673526	2.823286	2.767083
66	1	0	0.297068	2.907601	3.793150
67	1	0	1.400646	3.637059	2.659963
68	7	0	2.033807	-1.272228	-0.165867
69	7	0	1.924135	0.866025	1.500193
70	7	0	1.289523	2.036117	-1.218885
71	8	0	0.136234	-1.094982	-1.911082
72	8	0	1.033289	-2.692491	-3.240775
73	71	0	0.000072	0.075661	0.000081

E(RTPSSh) = -1682.06144382

Zero-point correction= 0.619686 (Hartree/Particle)

Thermal correction to Energy= 0.653411

Thermal correction to Enthalpy= 0.654356

Thermal correction to Gibbs Free Energy= 0.558918

Sum of electronic and zero-point Energies= -1681.441758

Sum of electronic and thermal Energies= -1681.408032

Sum of electronic and thermal Enthalpies= -1681.407088

Sum of electronic and thermal Free Energies= -1681.502526

Complejos de H_2cb-TEDPA

Las geometrías optimizadas en disolución se corresponden con las siguientes conformaciones:

- F1: Δ(λλ)(λ)
- F2: Δ(λδ)(λ)
- F3: Δ(δλ)(λ)
- F4: Δ(δδ)(λ)

Sin embargo, las formas 2, 3 y 4 revirtieron hacia la forma 1.

[La(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.768479	-2.031876	-2.267792
2	6	0	-2.791807	-1.955691	-1.141718
3	6	0	-4.044407	-2.563968	-1.225233
4	1	0	-4.309801	-3.111799	-2.121757
5	6	0	-4.917559	-2.437835	-0.142425
6	1	0	-5.903453	-2.890644	-0.177206
7	6	0	-4.517616	-1.720167	0.989223
8	1	0	-5.178590	-1.607407	1.841900
9	6	0	-3.242652	-1.147911	1.004101
10	6	0	-2.662004	-0.417363	2.194405
11	1	0	-1.993191	-1.102611	2.729366
12	1	0	-3.458369	-0.118977	2.890434
13	6	0	-1.170898	1.262835	3.034023
14	1	0	-1.944837	1.535559	3.767385
15	1	0	-0.622595	0.405598	3.437136
16	6	0	-0.203982	2.453257	2.920000
17	1	0	0.011939	2.719143	3.962224
18	1	0	-0.698453	3.338794	2.508431
19	6	0	1.175544	2.246415	2.268942
20	1	0	1.833339	3.057185	2.620347
21	1	0	1.609401	1.306304	2.626442
22	6	0	2.610680	1.990078	0.329145

23	1	0	2.975485	1.100004	0.849482
24	1	0	3.259529	2.828254	0.630487
25	6	0	2.754940	1.806871	-1.189614
26	1	0	3.800895	1.543894	-1.387337
27	1	0	2.583464	2.751923	-1.709331
28	6	0	1.173613	1.262104	-3.034094
29	1	0	1.948024	1.534181	-3.767197
30	1	0	0.624252	0.405803	-3.437813
31	6	0	0.208214	2.453704	-2.919561
32	1	0	0.703863	3.338484	-2.507790
33	1	0	-0.007590	2.720177	-3.961655
34	6	0	-1.171450	2.248288	-2.268309
35	1	0	-1.606403	1.308717	-2.625966
36	1	0	-1.828408	3.059837	-2.619424
37	6	0	-2.607118	1.994923	-0.328422
38	1	0	-2.974545	1.106294	-0.849339
39	1	0	-3.253712	2.835028	-0.629132
40	6	0	-2.751715	1.810862	1.190189
41	1	0	-2.578848	2.755280	1.710585
42	1	0	-3.798066	1.549305	1.387685
43	6	0	2.661892	-0.420758	-2.194485
44	1	0	3.458824	-0.123596	-2.890388
45	1	0	1.992214	-1.105127	-2.729492
46	6	0	3.241228	-1.151701	-1.003804
47	6	0	4.515866	-1.724621	-0.987843
48	1	0	5.177507	-1.612444	-1.840080
49	6	0	4.914658	-2.442071	0.144353
50	1	0	5.900343	-2.895266	0.180052
51	6	0	4.040617	-2.567447	1.226520
52	1	0	4.305047	-3.115120	2.123426
53	6	0	2.788398	-1.958514	1.141918
54	6	0	1.764252	-2.033844	2.267319
55	6	0	-0.730214	3.526892	-0.222575
56	1	0	-1.364510	3.784282	0.623805
57	1	0	-0.878468	4.326234	-0.962255
58	6	0	0.736599	3.525847	0.223336

59	1	0	1.371318	3.782394	-0.622989
60	1	0	0.885898	4.325008	0.963026
61	7	0	-2.415887	-1.265602	-0.049677
62	7	0	-1.850468	0.770769	1.789259
63	7	0	-1.202787	2.229403	-0.775120
64	7	0	1.207087	2.227723	0.775860
65	7	0	1.852119	0.768556	-1.789413
66	7	0	2.413642	-1.268469	0.049447
67	8	0	-0.653598	-1.404002	-2.038710
68	8	0	-2.055410	-2.666662	-3.288945
69	8	0	0.650473	-1.404179	2.037947
70	8	0	2.049638	-2.669679	3.288262
71	57	0	-0.000629	-0.190615	-0.000870

E(RTPSSh) = -1672.48815859

Zero-point correction= 0.597657 (Hartree/Particle)

Thermal correction to Energy= 0.629503

Thermal correction to Enthalpy= 0.630447

Thermal correction to Gibbs Free Energy= 0.537820

Sum of electronic and zero-point Energies= -1671.890501

Sum of electronic and thermal Energies= -1671.858656

Sum of electronic and thermal Enthalpies= -1671.857712

Sum of electronic and thermal Free Energies= -1671.950338

[Nd(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.420953	-2.038262	-2.298241
2	6	0	-2.516151	-2.025758	-1.241802
3	6	0	-3.710172	-2.731390	-1.385034
4	1	0	-3.876692	-3.317756	-2.280945

5	6	0	-4.656732	-2.648312	-0.360794
6	1	0	-5.601401	-3.176577	-0.442645
7	6	0	-4.383893	-1.876202	0.771910
8	1	0	-5.103655	-1.795309	1.579474
9	6	0	-3.159090	-1.207022	0.849975
10	6	0	-2.710371	-0.420625	2.059020
11	1	0	-2.055020	-1.065611	2.655324
12	1	0	-3.571607	-0.142239	2.681903
13	6	0	-1.330371	1.307406	2.973718
14	1	0	-2.155275	1.590434	3.644855
15	1	0	-0.809621	0.458780	3.426644
16	6	0	-0.355797	2.493060	2.905661
17	1	0	-0.196094	2.768808	3.955363
18	1	0	-0.819793	3.376867	2.456507
19	6	0	1.052188	2.259299	2.332412
20	1	0	1.708961	3.056495	2.713912
21	1	0	1.445157	1.309253	2.711447
22	6	0	2.583204	1.974131	0.474453
23	1	0	2.895237	1.072067	1.010166
24	1	0	3.229339	2.795606	0.822254
25	6	0	2.811804	1.799221	-1.034685
26	1	0	3.860345	1.510740	-1.174127
27	1	0	2.694157	2.752290	-1.555102
28	6	0	1.331610	1.306412	-2.973959
29	1	0	2.156776	1.588896	-3.645019
30	1	0	0.810315	0.458182	-3.426983
31	6	0	0.357857	2.492735	-2.905965
32	1	0	0.822487	3.376160	-2.456748
33	1	0	0.198311	2.768680	-3.955649
34	6	0	-1.050330	2.259896	-2.332689
35	1	0	-1.443792	1.310019	-2.711594
36	1	0	-1.706607	3.057402	-2.714357
37	6	0	-2.581584	1.975970	-0.474611
38	1	0	-2.894193	1.074006	-1.010260
39	1	0	-3.227214	2.797782	-0.822566
40	6	0	-2.810170	1.801464	1.034537

41	1	0	-2.691364	2.754510	1.554730
42	1	0	-3.858999	1.514194	1.174314
43	6	0	2.709891	-0.422897	-2.059006
44	1	0	3.571298	-0.145501	-2.682081
45	1	0	2.053854	-1.067458	-2.655033
46	6	0	3.158078	-1.209233	-0.849723
47	6	0	4.382478	-1.879125	-0.771397
48	1	0	5.102179	-1.799171	-1.579101
49	6	0	4.654983	-2.650725	0.361747
50	1	0	5.599358	-3.179488	0.443807
51	6	0	3.708476	-2.732638	1.386114
52	1	0	3.874752	-3.318456	2.282433
53	6	0	2.514762	-2.026521	1.242485
54	6	0	1.419444	-2.037891	2.298843
55	6	0	-0.720852	3.534852	-0.259114
56	1	0	-1.397794	3.782462	0.555965
57	1	0	-0.835115	4.337510	-1.000637
58	6	0	0.723818	3.534150	0.258569
59	1	0	1.400815	3.780764	-0.556769
60	1	0	0.839130	4.337000	0.999765
61	7	0	-2.260289	-1.285617	-0.146910
62	7	0	-1.916294	0.790649	1.691766
63	7	0	-1.158343	2.237006	-0.842490
64	7	0	1.160221	2.236104	0.842223
65	7	0	1.916987	0.789222	-1.691921
66	7	0	2.259239	-1.286865	0.147207
67	8	0	-0.380994	-1.308734	-2.013688
68	8	0	-1.581911	-2.714838	-3.319019
69	8	0	0.379550	-1.308739	2.013263
70	8	0	1.580258	-2.713401	3.320355
71	60	0	-0.000281	-0.060185	-0.000337

E(RTPSSh) = -1674.39795487

Zero-point correction= 0.598331 (Hartree/Particle)

Thermal correction to Energy= 0.629951

Thermal correction to Enthalpy= 0.630895

Thermal correction to Gibbs Free Energy= 0.539382

Sum of electronic and zero-point Energies= -1673.799624

Sum of electronic and thermal Energies= -1673.768004

Sum of electronic and thermal Enthalpies= -1673.767060

Sum of electronic and thermal Free Energies= -1673.858573

[Eu(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.301335	-2.017337	-2.302347
2	6	0	-2.418094	-2.032345	-1.272706
3	6	0	-3.594121	-2.761278	-1.440755
4	1	0	-3.730689	-3.349997	-2.340234
5	6	0	-4.562966	-2.696762	-0.436076
6	1	0	-5.495685	-3.242671	-0.537090
7	6	0	-4.327283	-1.919660	0.701226
8	1	0	-5.064521	-1.851971	1.494117
9	6	0	-3.117594	-1.226410	0.803819
10	6	0	-2.707723	-0.430504	2.017893
11	1	0	-2.057127	-1.065011	2.629353
12	1	0	-3.585519	-0.157161	2.619267
13	6	0	-1.366319	1.310239	2.953289
14	1	0	-2.208825	1.591557	3.602881
15	1	0	-0.852748	0.465237	3.419853
16	6	0	-0.394929	2.497503	2.902842
17	1	0	-0.252203	2.774916	3.954586
18	1	0	-0.851650	3.380245	2.444014
19	6	0	1.019201	2.258390	2.350895
20	1	0	1.673413	3.057482	2.732456
21	1	0	1.405155	1.309967	2.740334
22	6	0	2.570471	1.959404	0.514410

23	1	0	2.871778	1.055328	1.051934
24	1	0	3.212616	2.778959	0.873543
25	6	0	2.816492	1.787295	-0.991131
26	1	0	3.863829	1.489932	-1.119843
27	1	0	2.713006	2.742478	-1.510608
28	6	0	1.366093	1.309914	-2.953581
29	1	0	2.208506	1.591393	-3.603224
30	1	0	0.852757	0.464692	-3.420009
31	6	0	0.394321	2.496890	-2.903248
32	1	0	0.850824	3.379806	-2.444555
33	1	0	0.251449	2.774155	-3.954996
34	6	0	-1.019702	2.257410	-2.351179
35	1	0	-1.405260	1.308660	-2.740229
36	1	0	-1.674253	3.056044	-2.733125
37	6	0	-2.571047	1.958843	-0.514680
38	1	0	-2.872114	1.054635	-1.052113
39	1	0	-3.213299	2.778235	-0.873979
40	6	0	-2.816986	1.786864	0.990904
41	1	0	-2.713736	2.742152	1.510218
42	1	0	-3.864223	1.489189	1.119748
43	6	0	2.708040	-0.430237	-2.017750
44	1	0	3.585867	-0.156685	-2.618977
45	1	0	2.057813	-1.065058	-2.629281
46	6	0	3.117949	-1.225911	-0.803510
47	6	0	4.327455	-1.919542	-0.701070
48	1	0	5.064531	-1.852217	-1.494142
49	6	0	4.563149	-2.696497	0.436303
50	1	0	5.495746	-3.242626	0.537255
51	6	0	3.594435	-2.760659	1.441167
52	1	0	3.731009	-3.349356	2.340663
53	6	0	2.418565	-2.031508	1.273216
54	6	0	1.301686	-2.016575	2.302716
55	6	0	-0.718406	3.521202	-0.269208
56	1	0	-1.407618	3.765310	0.536245
57	1	0	-0.824143	4.324364	-1.011135
58	6	0	0.717585	3.521386	0.268515

59	1	0	1.406785	3.765355	-0.536989
60	1	0	0.823204	4.324757	1.010236
61	7	0	-2.196936	-1.286652	-0.173795
62	7	0	-1.918592	0.786429	1.659015
63	7	0	-1.143204	2.222708	-0.862059
64	7	0	1.142595	2.223086	0.861793
65	7	0	1.918473	0.786479	-1.659209
66	7	0	2.197494	-1.285740	0.174295
67	8	0	-0.288446	-1.262100	-1.986747
68	8	0	-1.417481	-2.692671	-3.329382
69	8	0	0.288480	-1.261865	1.986773
70	8	0	1.417956	-2.691593	3.329946
71	63	0	0.000140	-0.031605	-0.000014

E(RTPSSh) = -1676.21840351

Zero-point correction= 0.598972 (Hartree/Particle)

Thermal correction to Energy= 0.630428

Thermal correction to Enthalpy= 0.631372

Thermal correction to Gibbs Free Energy= 0.540494

Sum of electronic and zero-point Energies= -1675.619431

Sum of electronic and thermal Energies= -1675.587975

Sum of electronic and thermal Enthalpies= -1675.587031

Sum of electronic and thermal Free Energies= -1675.677910

[Gd(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.310767	-1.869571	2.378803
2	6	0	2.410776	-1.964177	1.337480
3	6	0	3.572076	-2.711596	1.522288
4	1	0	3.707812	-3.265596	2.443686

5	6	0	4.530191	-2.707897	0.504963
6	1	0	5.452749	-3.268477	0.618036
7	6	0	4.298060	-1.970494	-0.659052
8	1	0	5.028722	-1.947263	-1.460542
9	6	0	3.100899	-1.257455	-0.776905
10	6	0	2.695610	-0.494667	-2.012718
11	1	0	2.043297	-1.142438	-2.607790
12	1	0	3.575104	-0.239221	-2.619422
13	6	0	1.362215	1.226909	-2.991408
14	1	0	2.205924	1.491155	-3.646587
15	1	0	0.847963	0.371782	-3.438630
16	6	0	0.392109	2.415510	-2.968450
17	1	0	0.247872	2.668956	-4.025965
18	1	0	0.849430	3.308286	-2.530074
19	6	0	-1.020318	2.186443	-2.408525
20	1	0	-1.679122	2.970493	-2.812448
21	1	0	-1.401847	1.224251	-2.768442
22	6	0	-2.574024	1.942407	-0.568686
23	1	0	-2.877099	1.024894	-1.081668
24	1	0	-3.212289	2.754035	-0.951705
25	6	0	-2.821566	1.810880	0.939905
26	1	0	-3.868992	1.517332	1.076712
27	1	0	-2.716943	2.779360	1.434152
28	6	0	-1.377600	1.386424	2.914989
29	1	0	-2.223546	1.697755	3.546239
30	1	0	-0.876008	0.552588	3.411914
31	6	0	-0.392545	2.560062	2.834302
32	1	0	-0.837604	3.434913	2.349450
33	1	0	-0.249224	2.865390	3.878230
34	6	0	1.019733	2.288112	2.292432
35	1	0	1.389060	1.341720	2.701342
36	1	0	1.684322	3.087002	2.655938
37	6	0	2.572417	1.956946	0.459901
38	1	0	2.886030	1.072985	1.021530
39	1	0	3.206764	2.793368	0.793036
40	6	0	2.813671	1.746918	-1.041924

41	1	0	2.710742	2.689785	-1.583456
42	1	0	3.859978	1.444404	-1.167134
43	6	0	-2.711539	-0.380314	2.019497
44	1	0	-3.591776	-0.093509	2.610935
45	1	0	-2.062123	-0.997113	2.650118
46	6	0	-3.115349	-1.208900	0.825533
47	6	0	-4.325743	-1.902156	0.732678
48	1	0	-5.069799	-1.809304	1.516571
49	6	0	-4.552882	-2.712458	-0.383030
50	1	0	-5.486044	-3.258938	-0.476496
51	6	0	-3.574353	-2.810429	-1.375569
52	1	0	-3.703357	-3.426657	-2.257566
53	6	0	-2.397767	-2.079920	-1.218415
54	6	0	-1.268874	-2.103342	-2.234874
55	6	0	0.720162	3.507044	0.183856
56	1	0	1.411573	3.734234	-0.624629
57	1	0	0.827423	4.323478	0.910742
58	6	0	-0.714333	3.502860	-0.357723
59	1	0	-1.404870	3.771264	0.438809
60	1	0	-0.812697	4.287704	-1.119963
61	7	0	2.190414	-1.260557	0.211047
62	7	0	1.910475	0.733552	-1.684180
63	7	0	1.143174	2.218467	0.803708
64	7	0	-1.144226	2.192613	-0.918785
65	7	0	-1.922799	0.827902	1.632229
66	7	0	-2.186102	-1.300275	-0.141362
67	8	0	0.331066	-1.075663	2.049856
68	8	0	1.407352	-2.514766	3.426516
69	8	0	-0.253036	-1.348780	-1.929555
70	8	0	-1.379486	-2.807983	-3.242965
71	64	0	-0.005561	-0.028216	-0.005163

E(RTPSSh) = -1676.80852882

Zero-point correction= 0.598904 (Hartree/Particle)

Thermal correction to Energy= 0.630379

Thermal correction to Enthalpy= 0.631323

Thermal correction to Gibbs Free Energy= 0.540372

Sum of electronic and zero-point Energies= -1676.209624

Sum of electronic and thermal Energies= -1676.178150

Sum of electronic and thermal Enthalpies= -1676.177206

Sum of electronic and thermal Free Energies= -1676.268157

[Ho(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.216794	1.927997	-2.328354
2	6	0	2.331768	2.015551	-1.305506
3	6	0	3.476477	2.787705	-1.488349
4	1	0	3.586110	3.370103	-2.395617
5	6	0	4.452807	2.770598	-0.488648
6	1	0	5.363853	3.349881	-0.600830
7	6	0	4.253217	1.994434	0.655712
8	1	0	4.998224	1.958453	1.443423
9	6	0	3.070399	1.257681	0.772659
10	6	0	2.700793	0.449748	1.988774
11	1	0	2.053191	1.067981	2.618530
12	1	0	3.595265	0.184570	2.568806
13	6	0	1.412892	-1.315462	2.937757
14	1	0	2.274781	-1.617082	3.551797
15	1	0	0.923754	-0.474504	3.434512
16	6	0	0.424455	-2.486185	2.897612
17	1	0	0.294700	-2.771033	3.949075
18	1	0	0.857158	-3.372405	2.422152
19	6	0	-0.991233	-2.210552	2.370160
20	1	0	-1.659201	-2.997530	2.752212
21	1	0	-1.346768	-1.253697	2.766013
22	6	0	-2.568340	-1.920465	0.554007

23	1	0	-2.878547	-1.022864	1.095161
24	1	0	-3.190018	-2.751401	0.922016
25	6	0	-2.830636	-1.756430	-0.949186
26	1	0	-3.875228	-1.446348	-1.069913
27	1	0	-2.745298	-2.717136	-1.461995
28	6	0	-1.412838	-1.314598	-2.938239
29	1	0	-2.274719	-1.616090	-3.552355
30	1	0	-0.923745	-0.473474	-3.434768
31	6	0	-0.424314	-2.485266	-2.898402
32	1	0	-0.856974	-3.371658	-2.423223
33	1	0	-0.294489	-2.769799	-3.949936
34	6	0	0.991318	-2.209653	-2.370803
35	1	0	1.346726	-1.252579	-2.766254
36	1	0	1.659412	-2.996376	-2.753156
37	6	0	2.568474	-1.920224	-0.554610
38	1	0	2.878633	-1.022423	-1.095480
39	1	0	3.190121	-2.751031	-0.922936
40	6	0	2.830798	-1.756640	0.948635
41	1	0	2.745538	-2.717502	1.461164
42	1	0	3.875362	-1.446495	1.069427
43	6	0	-2.700806	0.450254	-1.988678
44	1	0	-3.595313	0.185169	-2.568702
45	1	0	-2.053319	1.068706	-2.618332
46	6	0	-3.070391	1.257818	-0.772305
47	6	0	-4.253075	1.994802	-0.655286
48	1	0	-4.997949	1.959277	-1.443144
49	6	0	-4.452690	2.770559	0.489330
50	1	0	-5.363630	3.349991	0.601604
51	6	0	-3.476512	2.787072	1.489212
52	1	0	-3.586198	3.369149	2.396683
53	6	0	-2.331923	2.014805	1.306246
54	6	0	-1.217060	1.926744	2.329157
55	6	0	0.712711	-3.464092	-0.281166
56	1	0	1.415038	-3.709482	0.511868
57	1	0	0.806138	-4.265534	-1.026036
58	6	0	-0.712526	-3.464226	0.280121

59	1	0	-1.414861	-3.709433	-0.512961
60	1	0	-0.805878	-4.265887	1.024766
61	7	0	2.140943	1.274287	-0.197320
62	7	0	1.923554	-0.775223	1.633263
63	7	0	1.130922	-2.163750	-0.881834
64	7	0	-1.130813	-2.164081	0.881227
65	7	0	-1.923471	-0.774761	-1.633581
66	7	0	-2.141091	1.273871	0.197813
67	8	0	0.261434	1.105084	-1.998759
68	8	0	1.278611	2.600186	-3.361214
69	8	0	-0.261405	1.104367	1.998999
70	8	0	-1.279164	2.598082	3.362544
71	67	0	-0.000020	0.005410	-0.000033

E(RTPSSh) = -1678.56889543

Zero-point correction= 0.599164 (Hartree/Particle)

Thermal correction to Energy= 0.630592

Thermal correction to Enthalpy= 0.631536

Thermal correction to Gibbs Free Energy= 0.540800

Sum of electronic and zero-point Energies= -1677.969731

Sum of electronic and thermal Energies= -1677.938304

Sum of electronic and thermal Enthalpies= -1677.937360

Sum of electronic and thermal Free Energies= -1678.028096

[Yb(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.133554	-1.901083	-2.333423
2	6	0	-2.261999	-2.014507	-1.331390
3	6	0	-3.387692	-2.808689	-1.532951
4	1	0	-3.470869	-3.392822	-2.441919

5	6	0	-4.380577	-2.810468	-0.549489
6	1	0	-5.278299	-3.407320	-0.675896
7	6	0	-4.214172	-2.029000	0.596299
8	1	0	-4.972265	-2.005263	1.371915
9	6	0	-3.047693	-1.269320	0.731647
10	6	0	-2.715055	-0.451612	1.949962
11	1	0	-2.078110	-1.060531	2.598562
12	1	0	-3.625042	-0.188366	2.506217
13	6	0	-1.460531	1.322712	2.916306
14	1	0	-2.336794	1.631358	3.505984
15	1	0	-0.987550	0.483448	3.430643
16	6	0	-0.465126	2.486319	2.892800
17	1	0	-0.351563	2.773691	3.945479
18	1	0	-0.882132	3.374054	2.406313
19	6	0	0.955464	2.194742	2.389907
20	1	0	1.624837	2.979043	2.774595
21	1	0	1.296644	1.237299	2.795747
22	6	0	2.559192	1.900839	0.598865
23	1	0	2.864038	1.001734	1.139870
24	1	0	3.169905	2.732991	0.981658
25	6	0	2.843927	1.746483	-0.900760
26	1	0	3.888100	1.430246	-1.008453
27	1	0	2.772713	2.711128	-1.408340
28	6	0	1.460591	1.322238	-2.916616
29	1	0	2.336878	1.630712	-3.506362
30	1	0	0.987534	0.482933	-3.430821
31	6	0	0.465266	2.485918	-2.893247
32	1	0	0.882349	3.373680	-2.406896
33	1	0	0.351658	2.773162	-3.945947
34	6	0	-0.955310	2.194465	-2.390249
35	1	0	-1.296525	1.236970	-2.795935
36	1	0	-1.624674	2.978722	-2.775025
37	6	0	-2.559107	1.900880	-0.599217
38	1	0	-2.863946	1.001707	-1.140119
39	1	0	-3.169715	2.733015	-0.982188
40	6	0	-2.843897	1.746759	0.900419

41	1	0	-2.772625	2.711462	1.407871
42	1	0	-3.888079	1.430560	1.008148
43	6	0	2.714950	-0.452011	-1.949961
44	1	0	3.624983	-0.188912	-2.506214
45	1	0	2.078017	-1.061004	-2.598496
46	6	0	3.047546	-1.269517	-0.731505
47	6	0	4.213896	-2.029429	-0.596190
48	1	0	4.971824	-2.006065	-1.371976
49	6	0	4.380375	-2.810619	0.549760
50	1	0	5.278002	-3.407621	0.676154
51	6	0	3.387659	-2.808397	1.533410
52	1	0	3.470905	-3.392301	2.442521
53	6	0	2.262063	-2.014111	1.331825
54	6	0	1.133694	-1.900406	2.333905
55	6	0	-0.707047	3.438814	-0.292931
56	1	0	-1.423017	3.683600	0.487624
57	1	0	-0.788149	4.240231	-1.038906
58	6	0	0.707211	3.438812	0.292476
59	1	0	1.423144	3.683485	-0.488150
60	1	0	0.788390	4.240328	1.038359
61	7	0	-2.101157	-1.268227	-0.221418
62	7	0	-1.938879	0.775878	1.602374
63	7	0	-1.114534	2.137807	-0.902982
64	7	0	1.114689	2.137871	0.902668
65	7	0	1.938860	0.775586	-1.602608
66	7	0	2.101173	-1.268016	0.221710
67	8	0	-0.204116	-1.058873	-1.979973
68	8	0	-1.159500	-2.567876	-3.371080
69	8	0	0.204032	-1.058573	1.980090
70	8	0	1.159846	-2.566671	3.371890
71	70	0	-0.000059	0.012506	0.000006

E(RTPSSh) = -1680.31563100

Zero-point correction= 0.599606 (Hartree/Particle)

Thermal correction to Energy= 0.630878

Thermal correction to Enthalpy= 0.631822

Thermal correction to Gibbs Free Energy= 0.541573

Sum of electronic and zero-point Energies= -1679.716025

Sum of electronic and thermal Energies= -1679.684753

Sum of electronic and thermal Enthalpies= -1679.683809

Sum of electronic and thermal Free Energies= -1679.774058

[Lu(cb-tedpa)]

F1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.093354	-1.909324	-2.325076
2	6	0	-2.237087	-2.015342	-1.341337
3	6	0	-3.359283	-2.811345	-1.553728
4	1	0	-3.430420	-3.399340	-2.461229
5	6	0	-4.363468	-2.811274	-0.581895
6	1	0	-5.258892	-3.409816	-0.716248
7	6	0	-4.209894	-2.026704	0.563420
8	1	0	-4.975451	-2.002546	1.331666
9	6	0	-3.046310	-1.264461	0.709146
10	6	0	-2.727443	-0.446710	1.930282
11	1	0	-2.098120	-1.056371	2.585261
12	1	0	-3.643094	-0.182176	2.476485
13	6	0	-1.477195	1.323378	2.907404
14	1	0	-2.356887	1.631826	3.492028
15	1	0	-1.008710	0.482647	3.423609
16	6	0	-0.480017	2.485107	2.891467
17	1	0	-0.371849	2.771988	3.944824
18	1	0	-0.891925	3.373762	2.402315
19	6	0	0.942077	2.188987	2.396322
20	1	0	1.612439	2.970377	2.784975
21	1	0	1.277530	1.230052	2.803550
22	6	0	2.556365	1.900800	0.614237

23	1	0	2.861927	1.001989	1.155247
24	1	0	3.161324	2.734849	1.001839
25	6	0	2.847960	1.750499	-0.884109
26	1	0	3.893118	1.436505	-0.988661
27	1	0	2.776848	2.715792	-1.390391
28	6	0	1.477338	1.322829	-2.907790
29	1	0	2.357075	1.631074	-3.492471
30	1	0	1.008769	0.482063	-3.423869
31	6	0	0.480258	2.484641	-2.891984
32	1	0	0.892261	3.373304	-2.402958
33	1	0	0.372021	2.771422	-3.945346
34	6	0	-0.941813	2.188626	-2.396702
35	1	0	-1.277261	1.229599	-2.803705
36	1	0	-1.612198	2.969921	-2.785486
37	6	0	-2.556217	1.900919	-0.614640
38	1	0	-2.861805	1.002056	-1.155548
39	1	0	-3.161001	2.734980	-1.002447
40	6	0	-2.847882	1.750878	0.883715
41	1	0	-2.776673	2.716224	1.389867
42	1	0	-3.893054	1.436944	0.988321
43	6	0	2.727309	-0.447220	-1.930301
44	1	0	3.643022	-0.182881	-2.476500
45	1	0	2.097983	-1.056941	-2.585211
46	6	0	3.046109	-1.264744	-0.709004
47	6	0	4.209543	-2.027259	-0.563321
48	1	0	4.974901	-2.003544	-1.331777
49	6	0	4.363211	-2.811494	0.582189
50	1	0	5.258521	-3.410214	0.716522
51	6	0	3.359222	-2.811040	1.554249
52	1	0	3.430448	-3.398749	2.461932
53	6	0	2.237133	-2.014926	1.341824
54	6	0	1.093483	-1.908606	2.325618
55	6	0	-0.704400	3.434392	-0.298747
56	1	0	-1.426355	3.681435	0.475469
57	1	0	-0.778947	4.234406	-1.046768
58	6	0	0.704683	3.434372	0.298223

59	1	0	1.426601	3.681250	-0.476084
60	1	0	0.779352	4.234509	1.046126
61	7	0	-2.089279	-1.262903	-0.233603
62	7	0	-1.946803	0.779355	1.589395
63	7	0	-1.108733	2.132406	-0.910041
64	7	0	1.108984	2.132464	0.909709
65	7	0	1.946810	0.778997	-1.589689
66	7	0	2.089263	-1.262709	0.233916
67	8	0	-0.165093	-1.073269	-1.953854
68	8	0	-1.104059	-2.575624	-3.362997
69	8	0	0.164947	-1.073024	1.953952
70	8	0	1.104443	-2.574264	3.363942
71	71	0	-0.000099	0.018168	0.000024

E(RTPSSh) = -1680.86935877

Zero-point correction= 0.599638 (Hartree/Particle)

Thermal correction to Energy= 0.630932

Thermal correction to Enthalpy= 0.631876

Thermal correction to Gibbs Free Energy= 0.541519

Sum of electronic and zero-point Energies= -1680.269721

Sum of electronic and thermal Energies= -1680.238427

Sum of electronic and thermal Enthalpies= -1680.237483

Sum of electronic and thermal Free Energies= -1680.327840