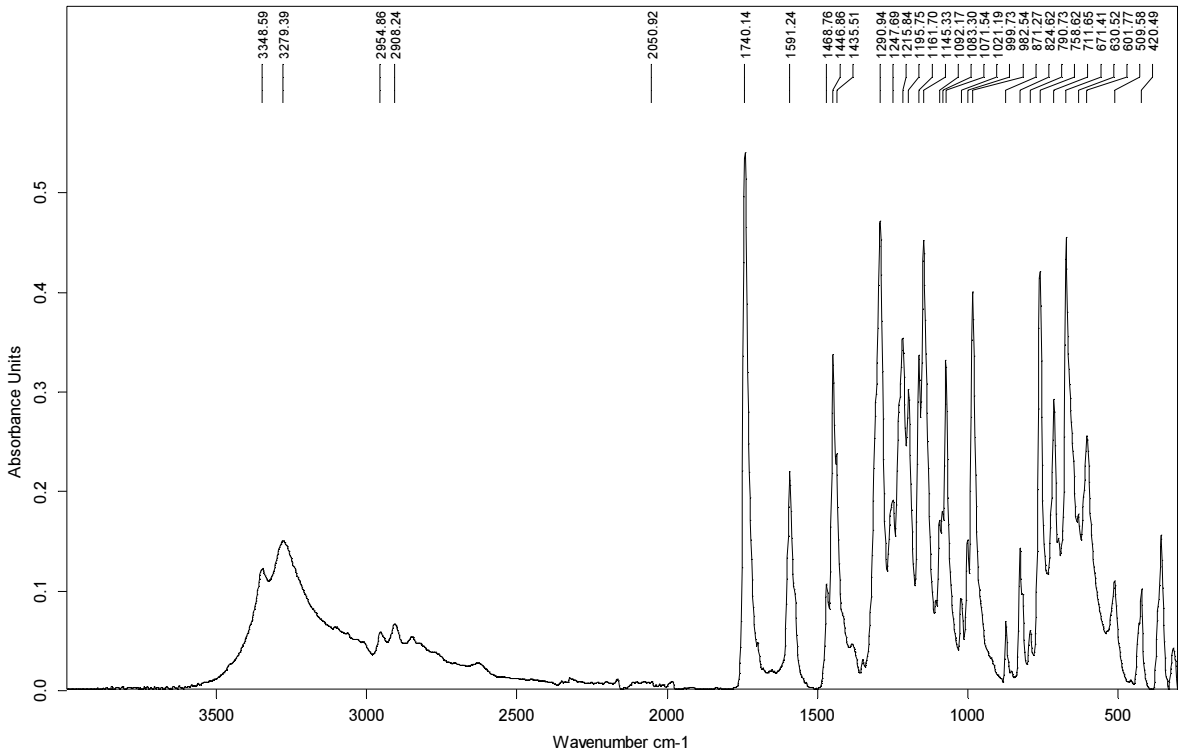
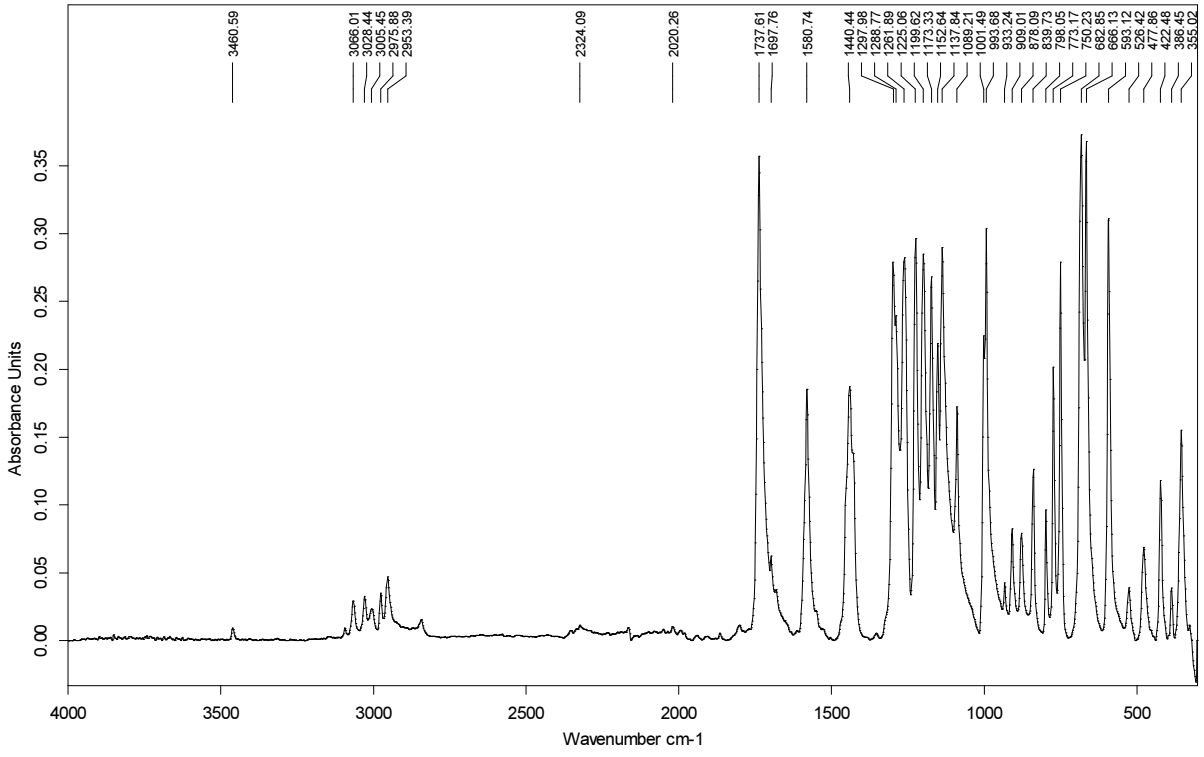
VI.1: ESPECTROS

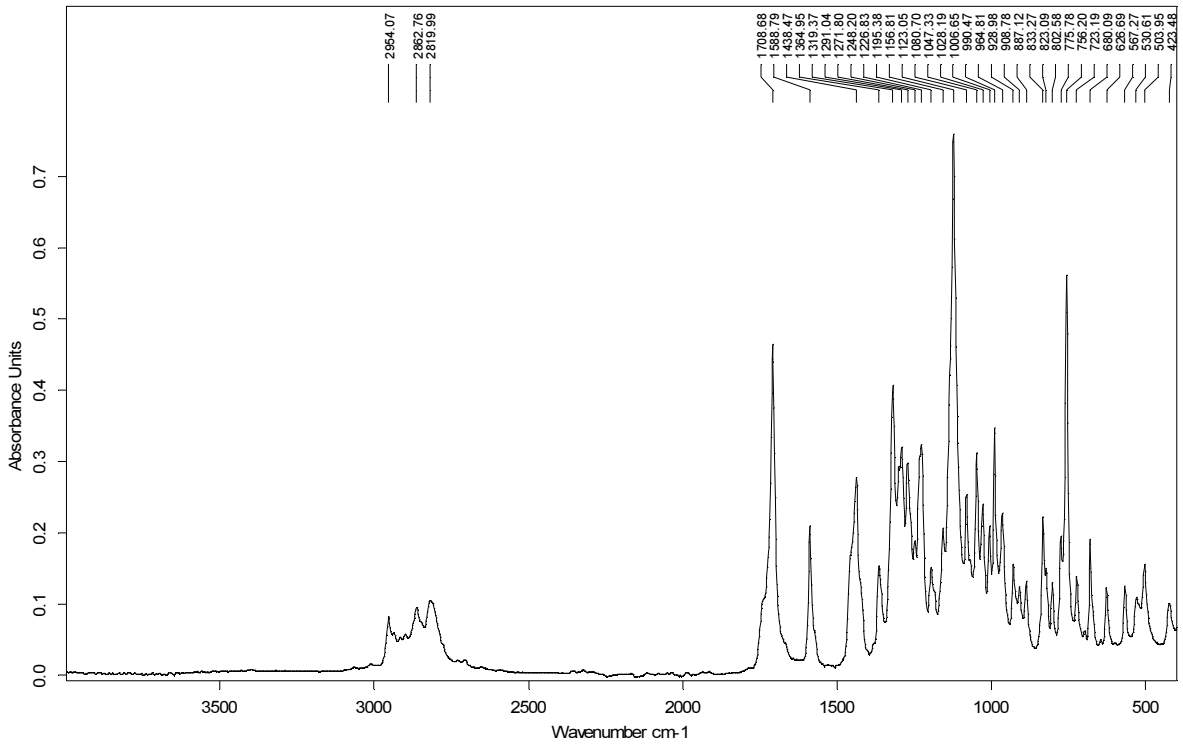
(2):


3348.59
3279.39
2954.86
2908.24
2050.92
1740.14
1591.24
1468.76
1446.86
1435.51
1290.94
1247.69
1215.84
1195.75
1161.70
1145.33
1092.17
1083.30
1071.54
1021.19
982.54
871.27
824.62
790.73
758.62
711.65
671.41
630.52
601.77
509.58
420.49
Absorbance Units
0.0
0.1
0.2
0.3
0.4
0.5
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

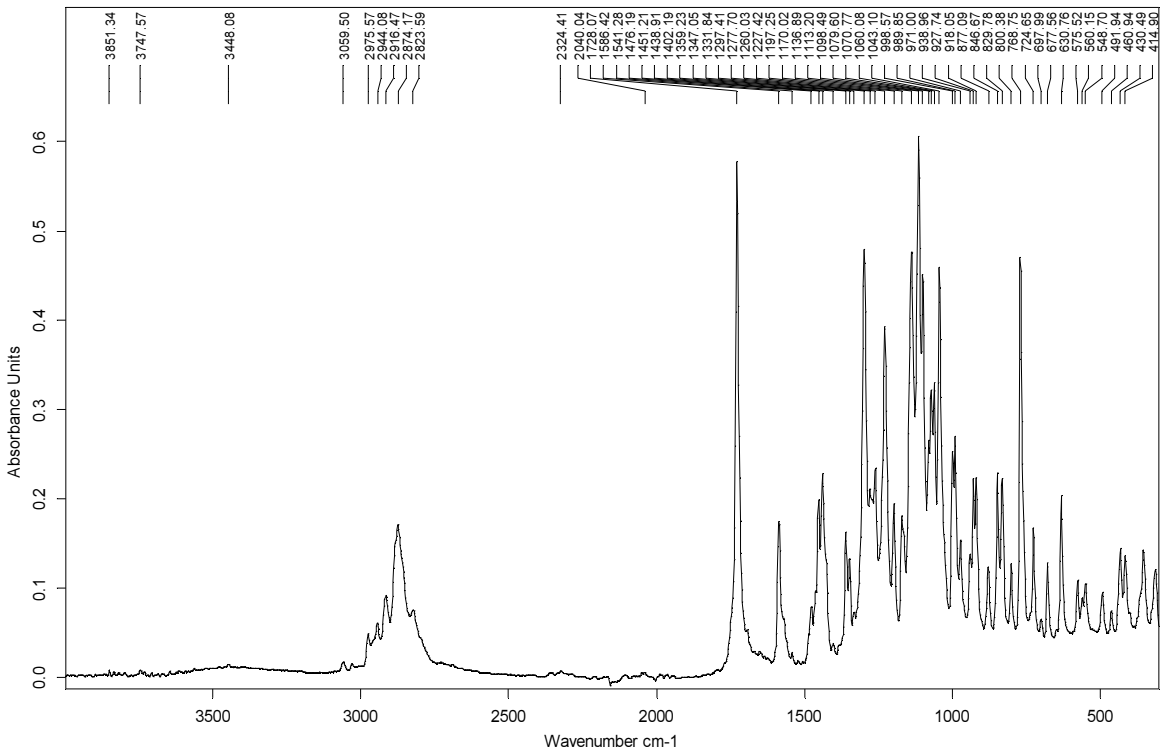
(3):


3460.59
3066.01
3028.44
3005.45
2975.88
2953.39
2324.09
2020.26
1737.61
1697.76
1580.74
1440.44
1297.98
1288.77
1261.89
1225.06
1199.62
1173.33
1152.64
1137.84
1089.21
1001.49
993.88
933.24
909.01
878.09
838.73
798.75
773.17
750.23
682.85
666.13
593.12
526.42
477.86
422.48
386.45
355.02
Absorbance Units
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

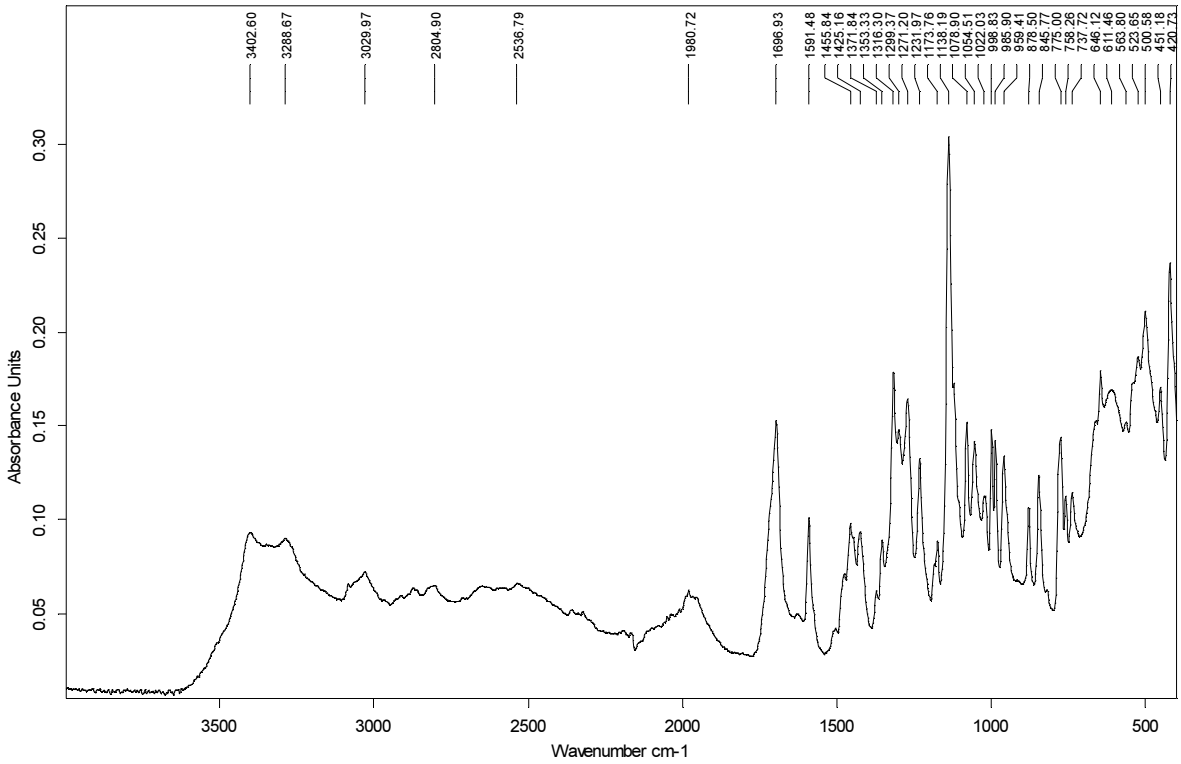
(4):


2954.07
2862.76
2819.99
1708.68
1588.79
1438.47
1364.95
1319.37
1291.04
1271.80
1248.20
1226.83
1195.38
1156.81
1123.05
1080.70
1047.33
1028.19
1006.65
990.47
964.81
938.88
908.78
887.12
833.27
823.09
802.58
775.78
756.20
723.19
680.09
625.69
567.27
530.61
503.95
423.48
Absorbance Units
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

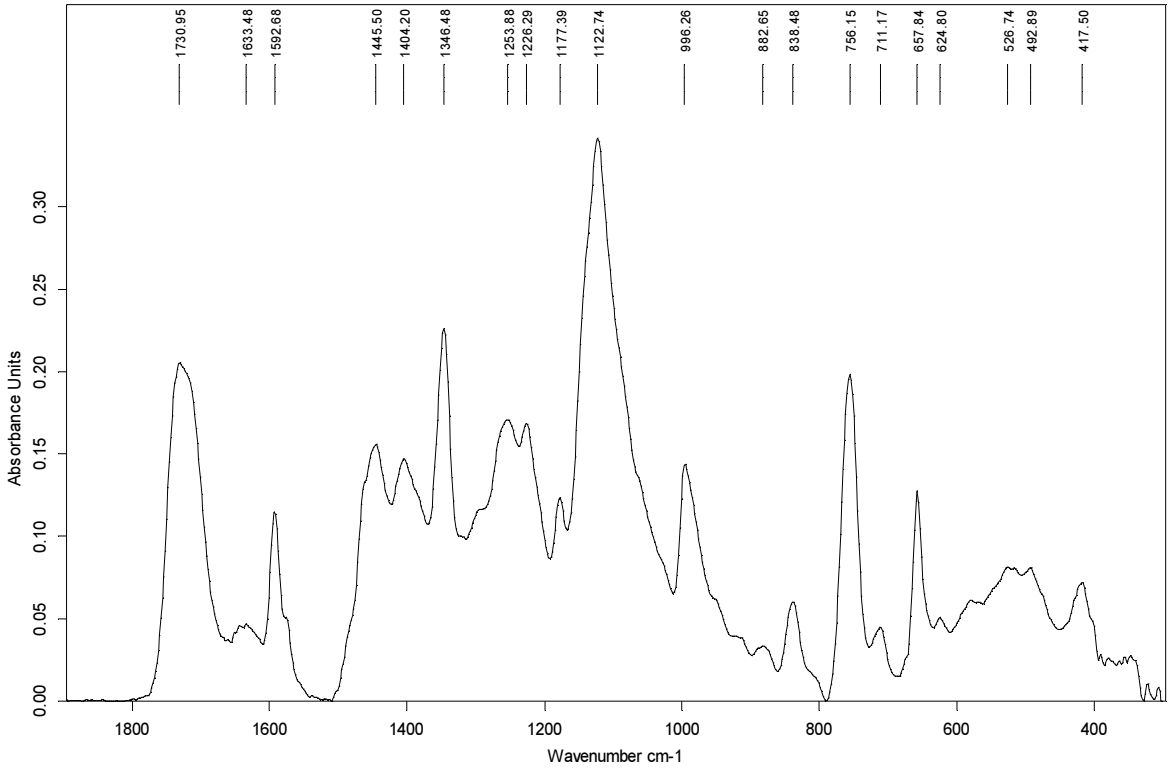
(6):


3851.34
3747.57
3448.08
3059.50
2975.57
2944.08
2916.47
2874.17
2823.59
2324.41
2040.04
1728.07
1586.42
1541.28
1495.19
1445.21
1438.91
1402.19
1359.23
1347.05
1331.84
1297.41
1277.70
1260.03
1227.42
1197.25
1170.02
1136.89
1113.20
1098.49
1079.60
1070.77
1060.08
1043.10
998.57
989.85
971.00
957.66
937.74
918.05
877.09
846.67
829.78
800.38
768.75
724.65
697.99
677.56
629.76
579.52
560.15
548.70
491.94
460.94
430.49
414.90
Absorbance Units
0.0
0.1
0.2
0.3
0.4
0.5
0.6
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

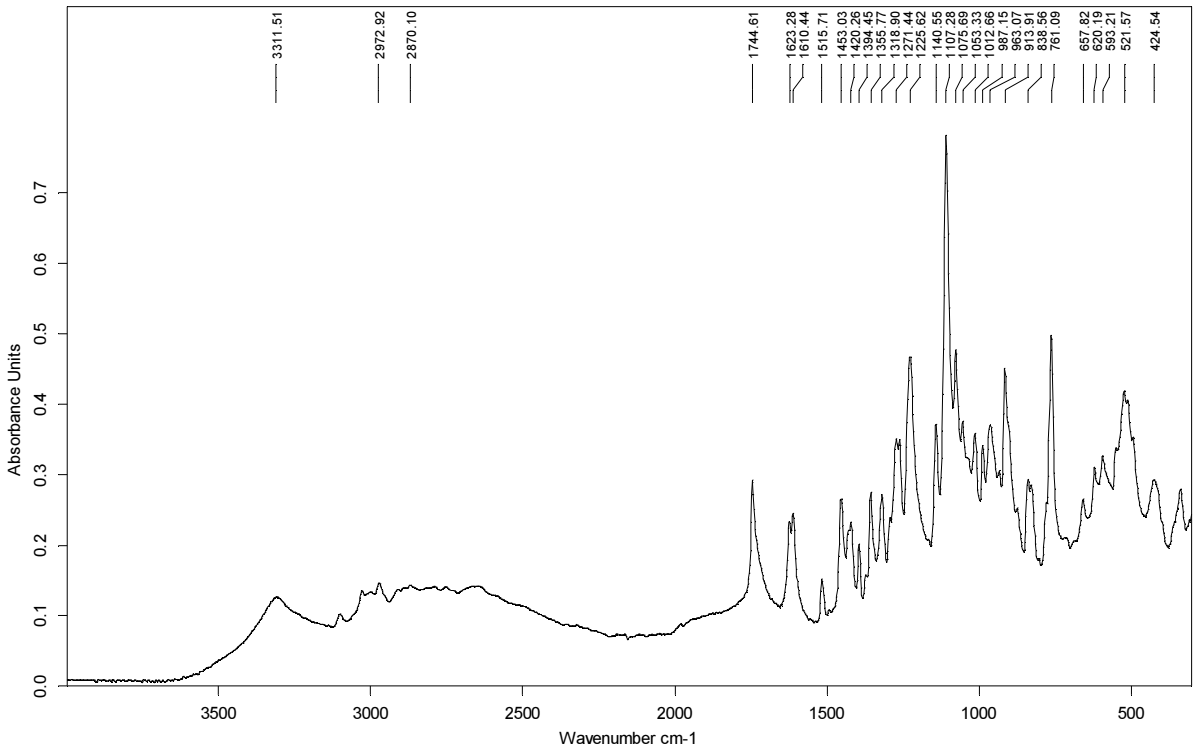
(H_2dpa12c4):



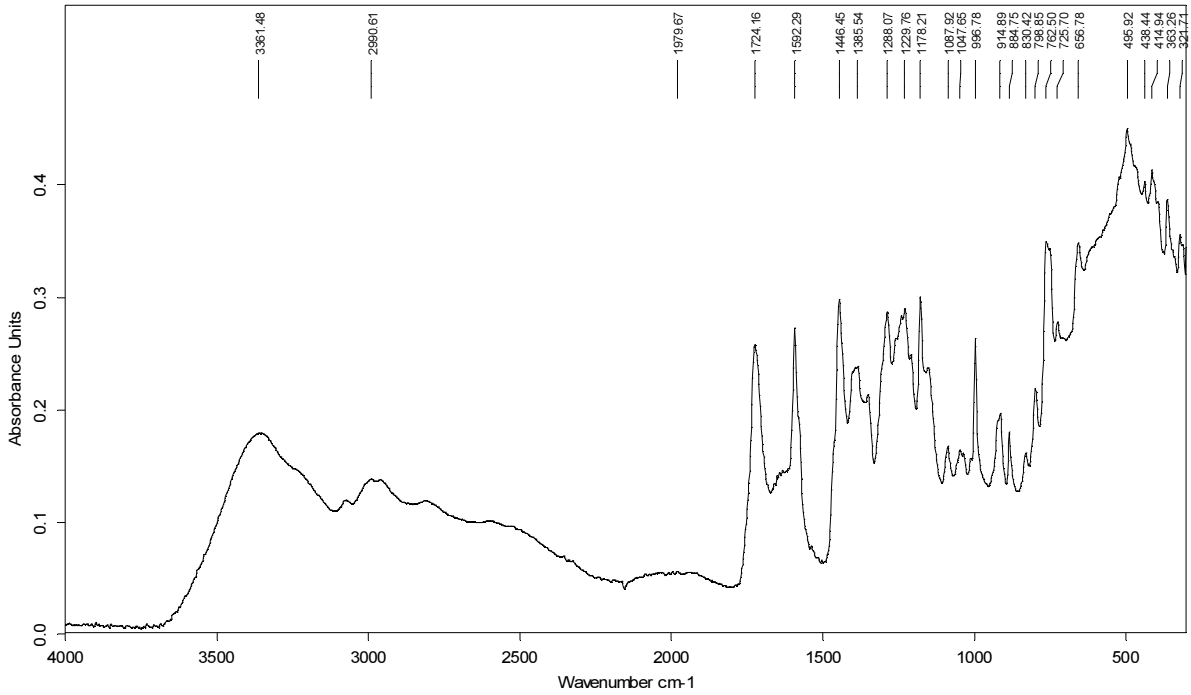
(H_2dpa15c5):



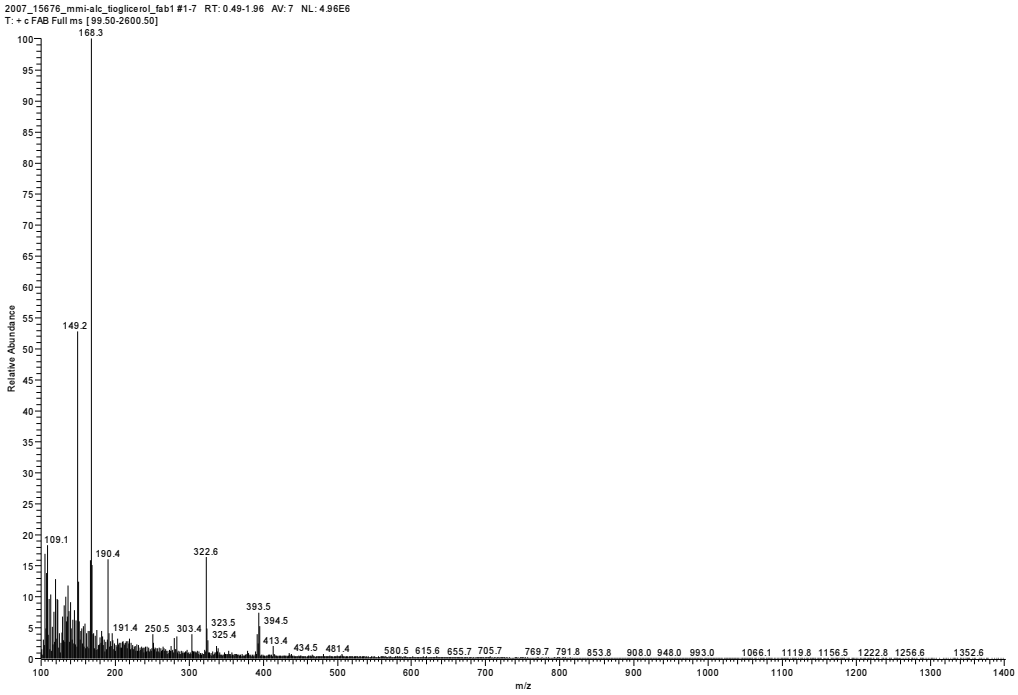
(H_2dpa18c6):



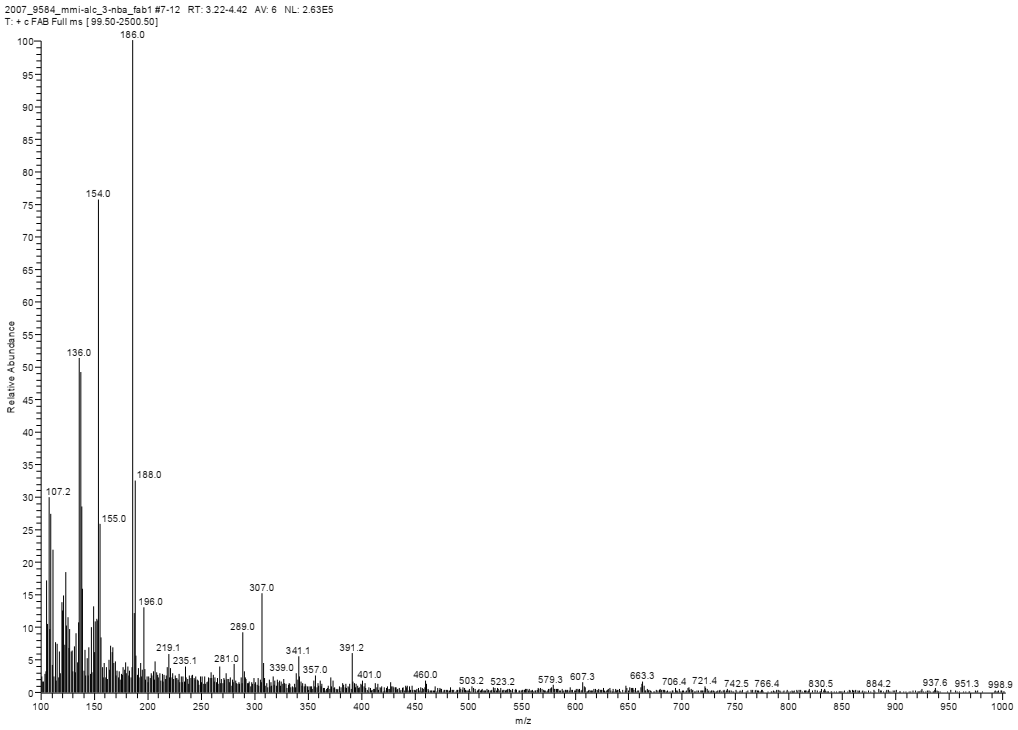
(H_2dpabp):



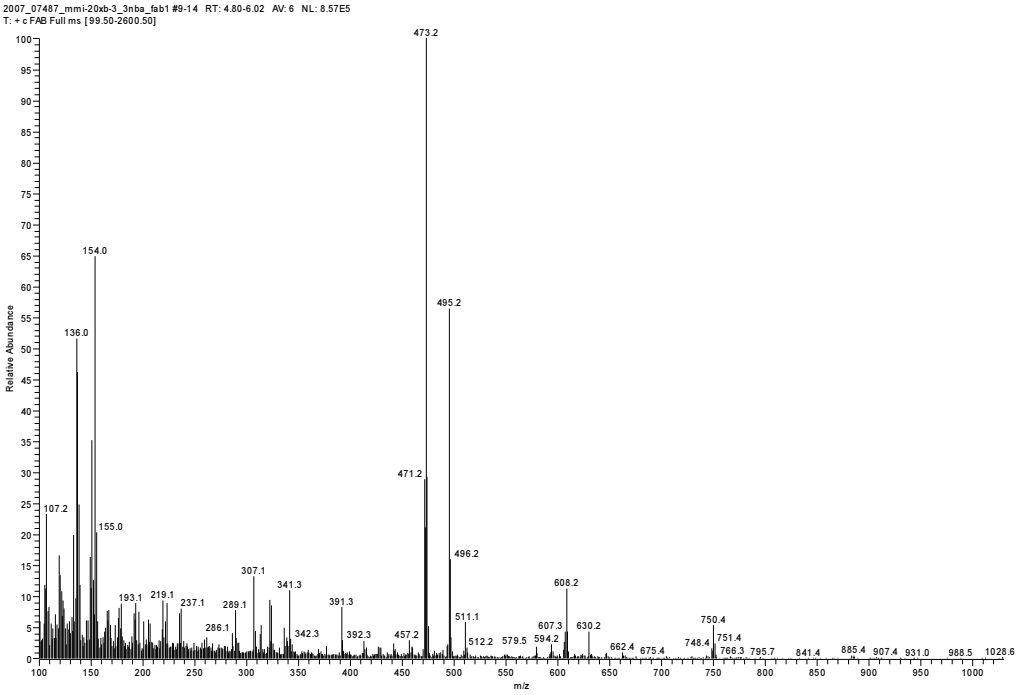
(2):


2007_15676_mmi-alc_tioglicerol_fab1 #1-7 RT: 0.49-1.96 AV: 7 NL: 4.96E6
T: + c FAB Full ms [99.50-2600.50]
Relative Abundance
m/z
168.3
149.2
109.1
190.4
322.6
393.5
394.5
323.5
325.4
191.4
250.5
303.4
413.4
434.5
481.4
580.5
615.6
655.7
705.7
769.7
791.8
853.8
908.0
948.0
993.0
1066.1
1119.8
1156.5
1222.8
1256.6
1352.6

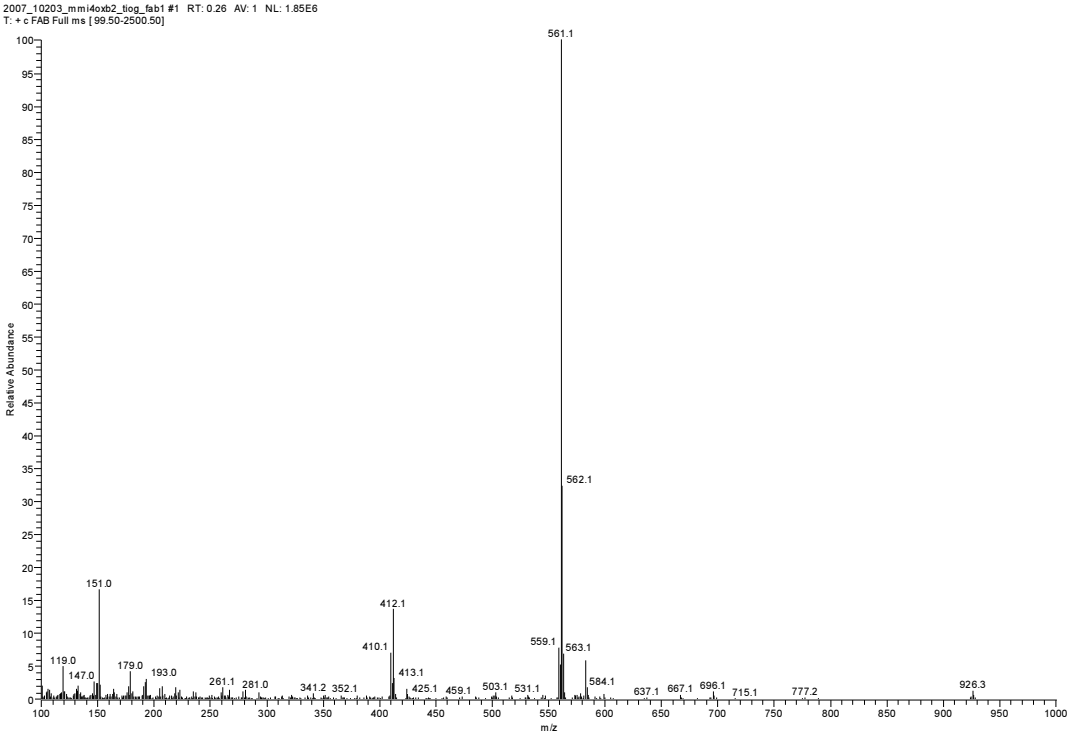
(3):


2007_9584_mmi-alc_3-nba_fab1 #7-12 RT: 3.22-4.42 AV: 6 NL: 2.63E5
T: + c FAB Full ms [99.50-2500.50]
Relative Abundance
m/z
186.0
154.0
136.0
188.0
107.2
155.0
307.0
196.0
289.0
341.1
391.2
219.1
235.1
281.0
339.0
357.0
401.0
460.0
503.2
523.2
579.3
607.3
663.3
706.4
721.4
742.5
766.4
830.5
884.2
937.6
951.3
998.9

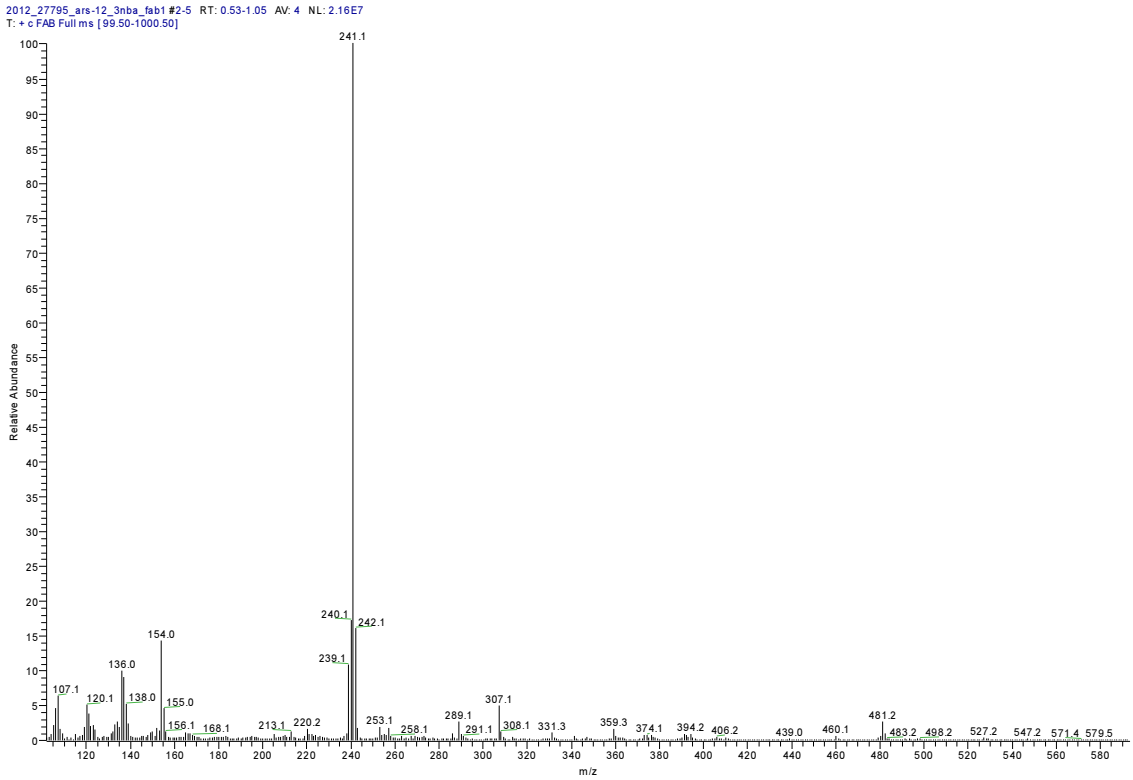
(4):


2007_07487_mmi-20xb-3_3nba_fab1 #9-14 RT: 4.80-6.02 AV: 6 NL: 8.57E5
T: + c FAB Full ms [99.50-2600.50]
Relative Abundance
m/z
473.2
495.2
154.0
136.0
471.2
107.2
155.0
496.2
608.2
307.1
341.3
391.3
193.1
219.1
237.1
289.1
511.1
750.4
751.4
607.3
630.2
286.1
342.3
392.3
457.2
512.2
579.5
594.2
662.4
675.4
748.4
766.3
795.7
841.4
885.4
907.4
931.0
988.5
1028.6

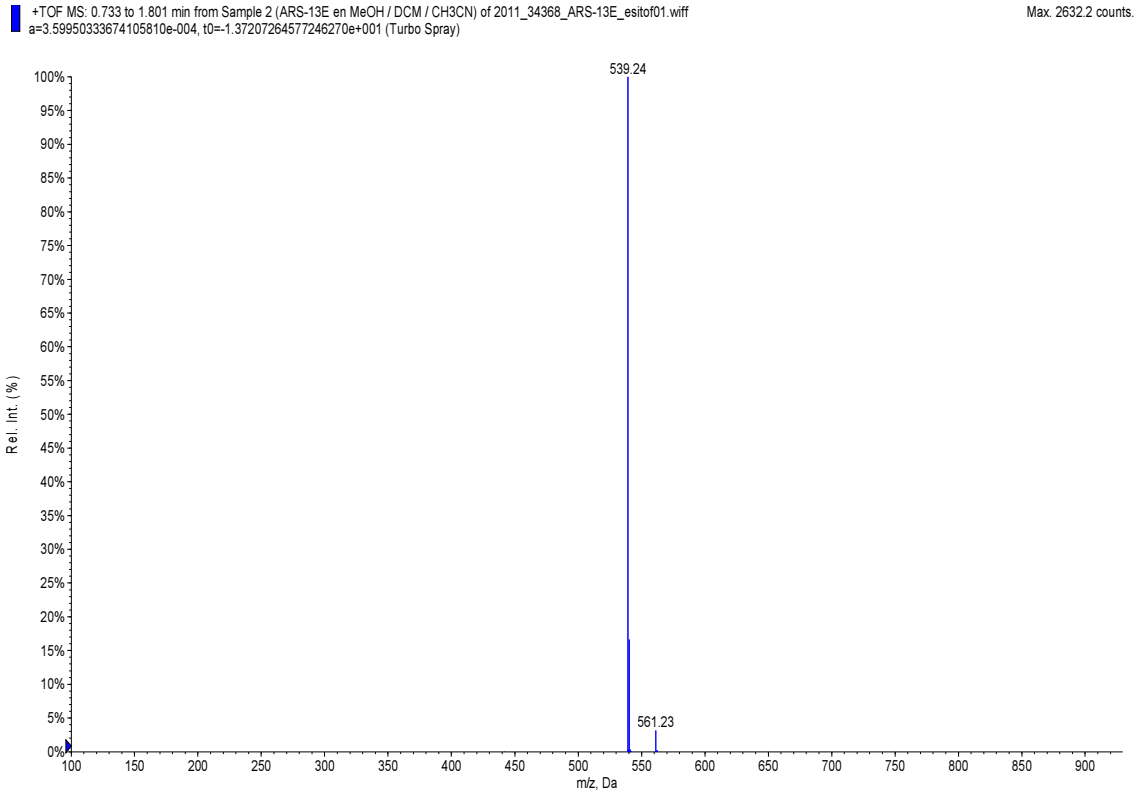
(6):


2007_10203_mmi4oxb2_tiog_fab1 #1 RT: 0.26 AV: 1 NL: 1.85E6
T: + c FAB Full ms [99.50-2500.50]
Relative Abundance
m/z
561.1
562.1
151.0
412.1
410.1
559.1
563.1
119.0
147.0
179.0
193.0
413.1
584.1
926.3

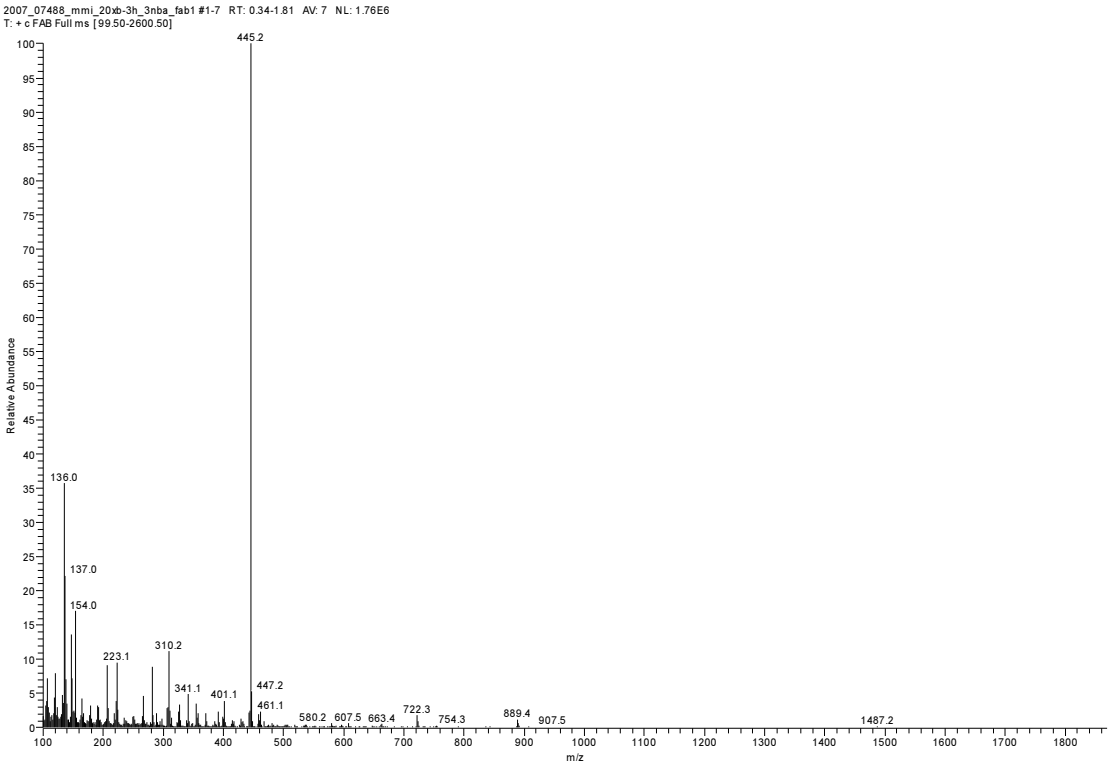
(7):


2012_27795_ars-12_3nba_fab1 #2-5 RT: 0.53-1.05 AV: 4 NL: 2.16E7
T: + c FAB Full ms [99.50-1000.50]
Relative Abundance
m/z
241.1
240.1
242.1
239.1
154.0
136.0
107.1
120.1
138.0
155.0
307.1
289.1
481.2

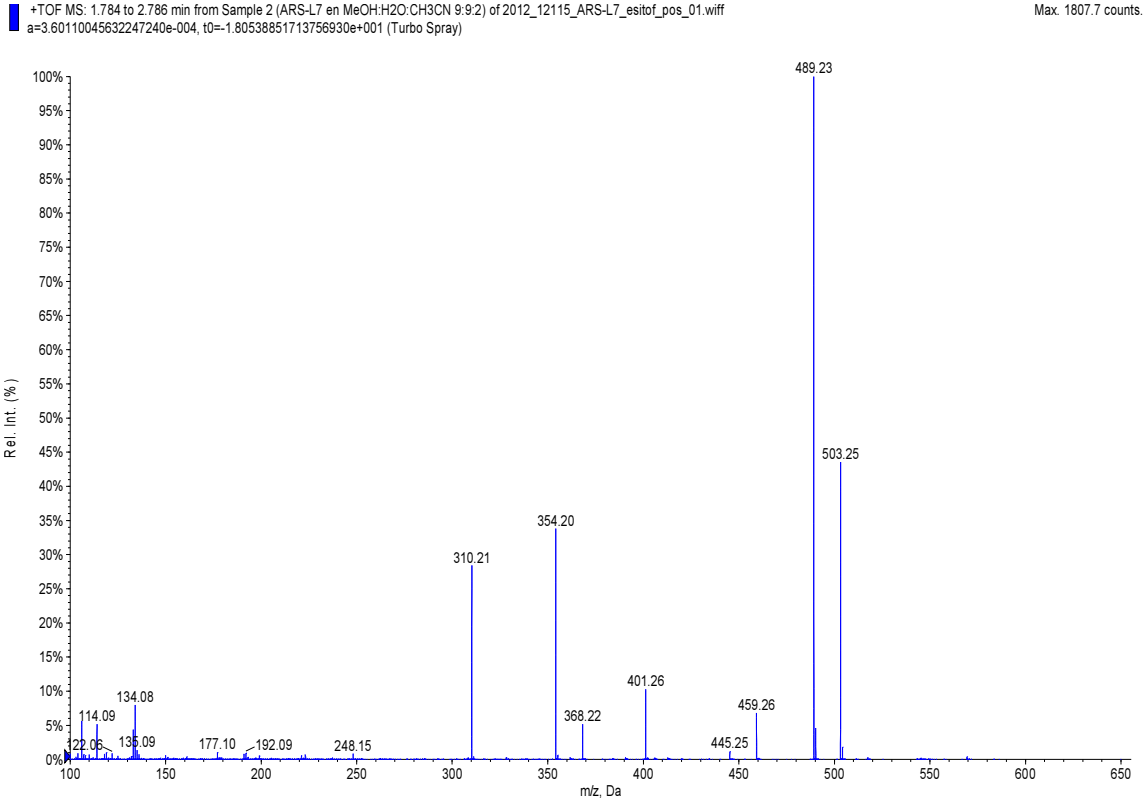
(9):


+TOF MS: 0.733 to 1.801 min from Sample 2 (ARS-13E en MeOH / DCM / CH3CN) of 2011_34368_ARS-13E_esitof01.wiff
a=3.59950333674105810e-004, t0=-1.37207264577246270e+001 (Turbo Spray)
Max. 2632.2 counts.
Rel. Int. (%)
m/z, Da
539.24
561.23

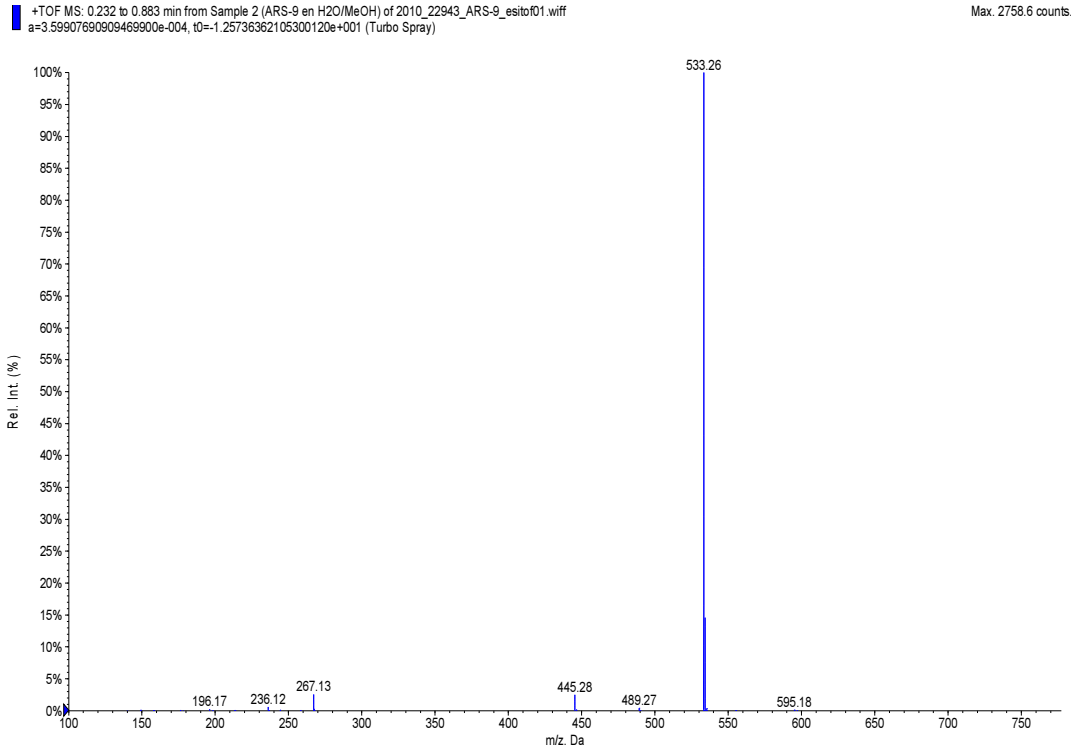
(H_2dpa12c4·HCl):



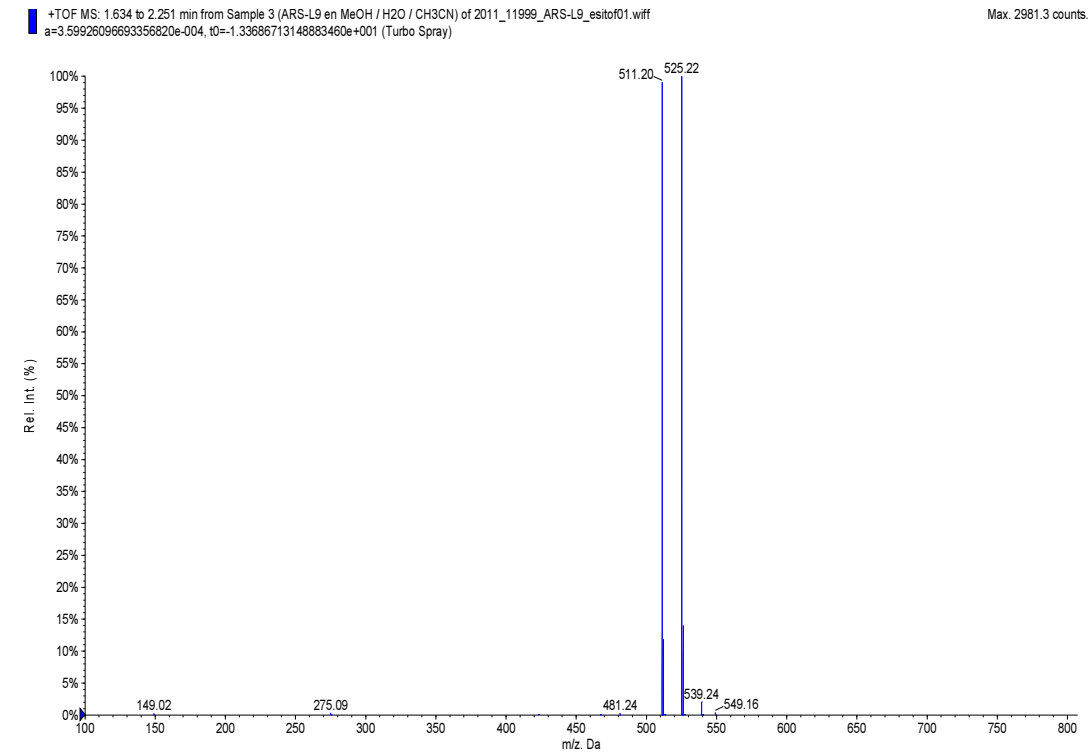
(H_2dpa15c5·4HCl·3H_2O):



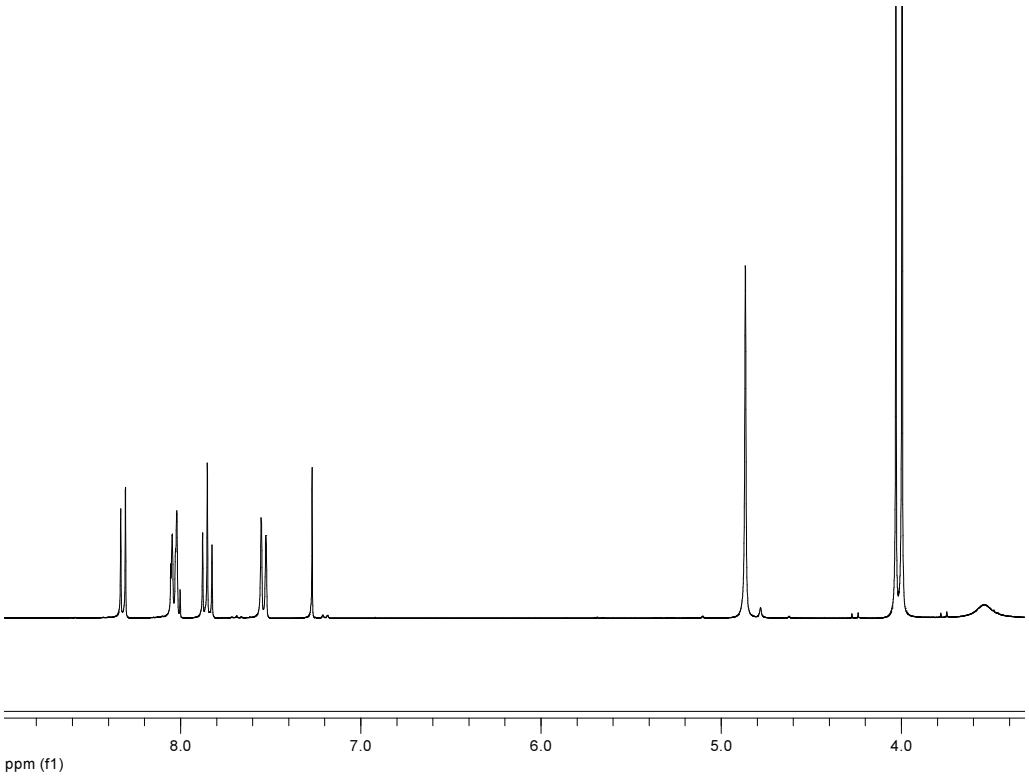
(H_2dpa18c6·2HCl·2H_2O):



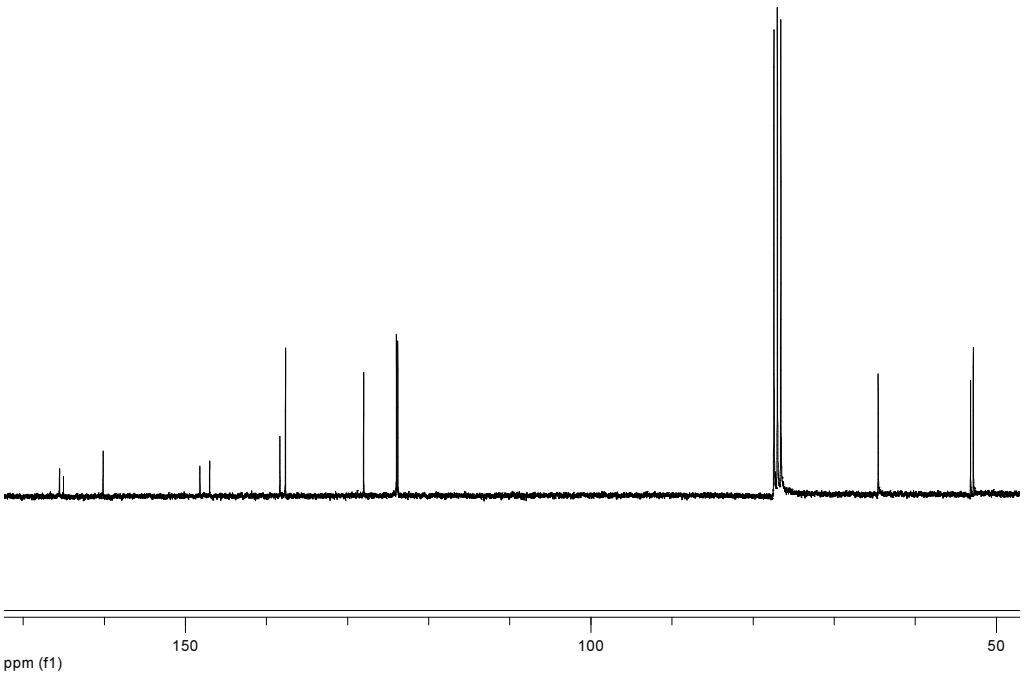
(H_2dpabp·7HCl·H_2O):



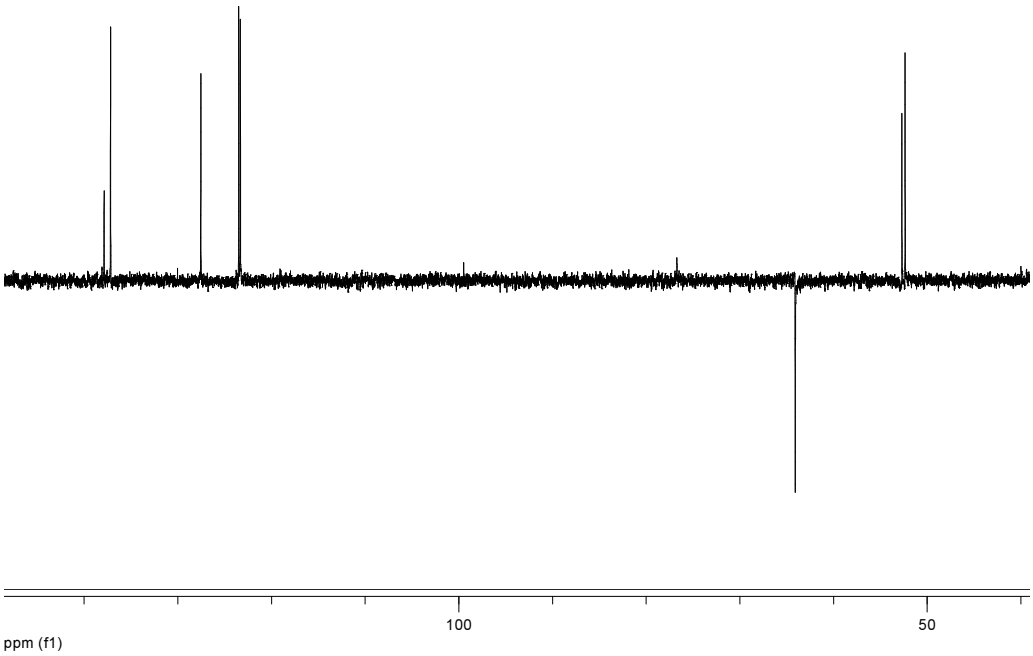
(2): ^{1}H-RMN ($CDCl_3$, 300 MHz) (δ / ppm)



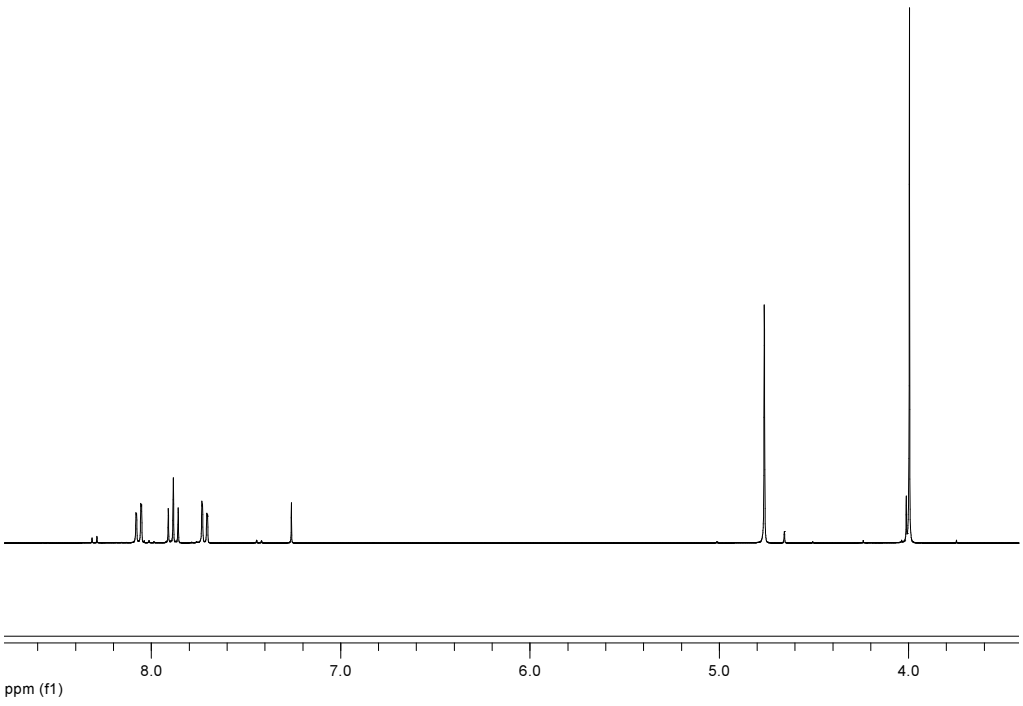
(2): ^{13}C-RMN ($CDCl_3$, 75.5 MHz) (δ / ppm)



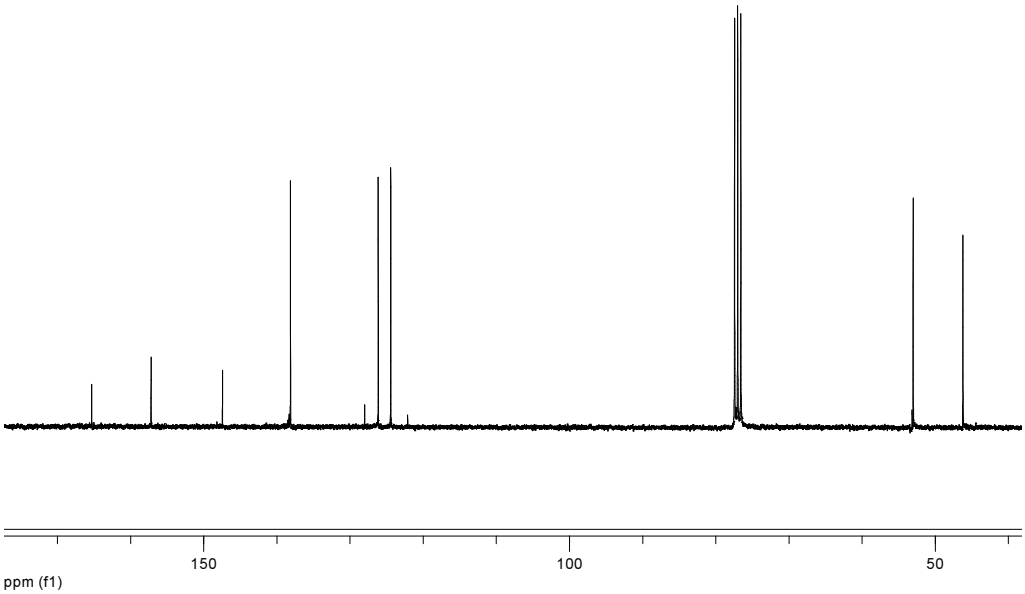
(2): ^{13}C- DEPT DCl_3, 75.5 MHz) (δ / ppm)



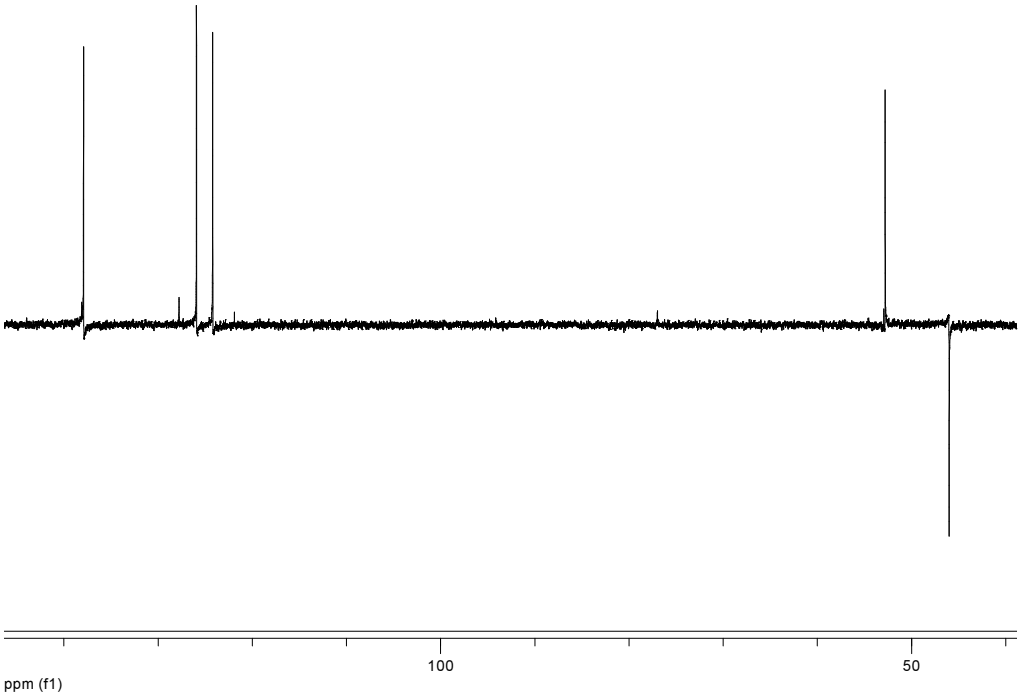
(3): ^{1}H-RMN ($CDCl_3$, 300 MHz) (δ / ppm)



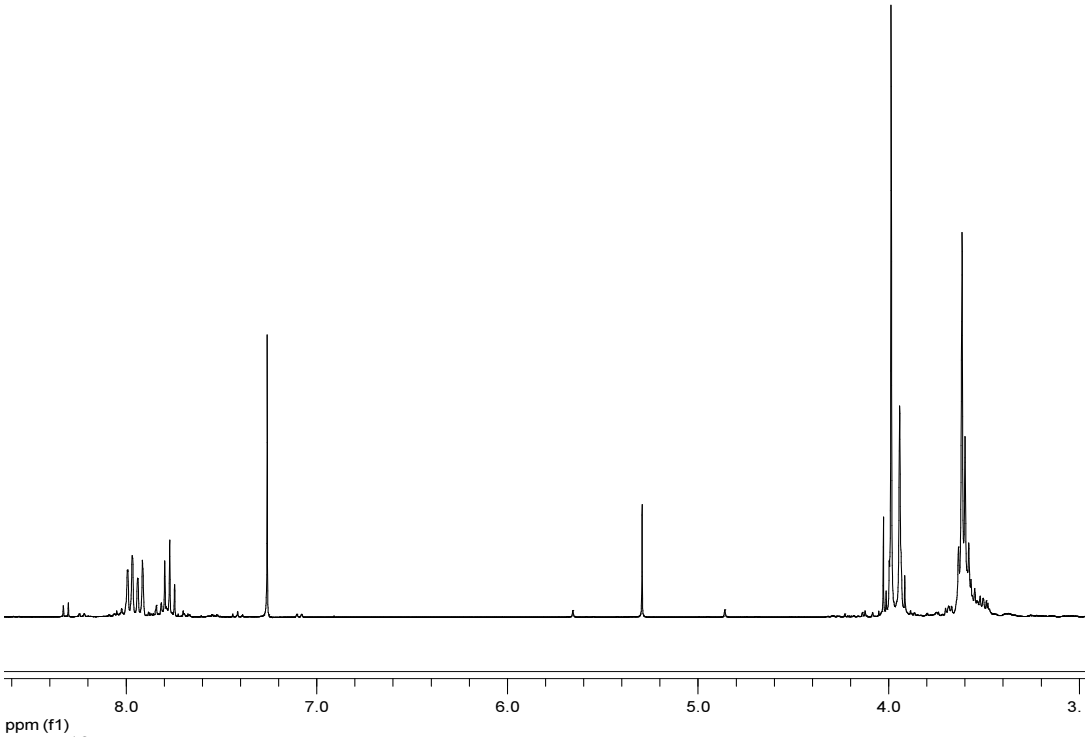
(3): ^{13}C-RMN ($CDCl_3$, 75.5 MHz) (δ / ppm)



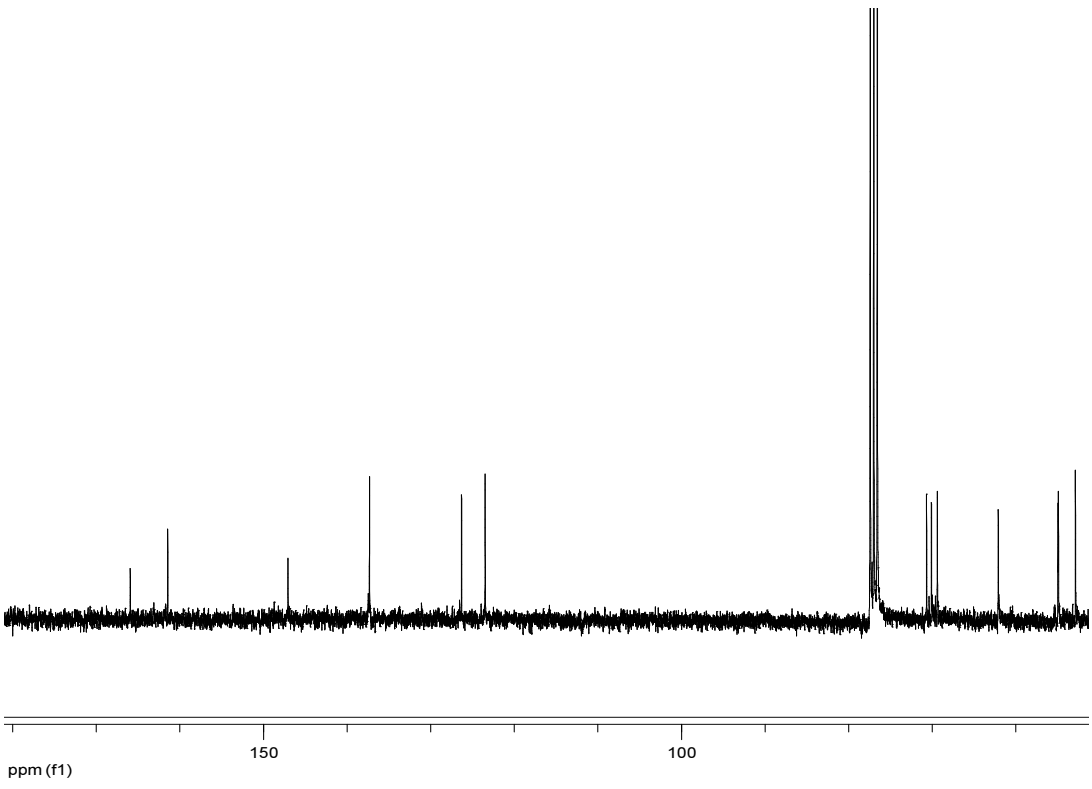
(3): ^{13}C- DEPT ($CDCl_3$, 75.5 MHz) (δ / ppm)



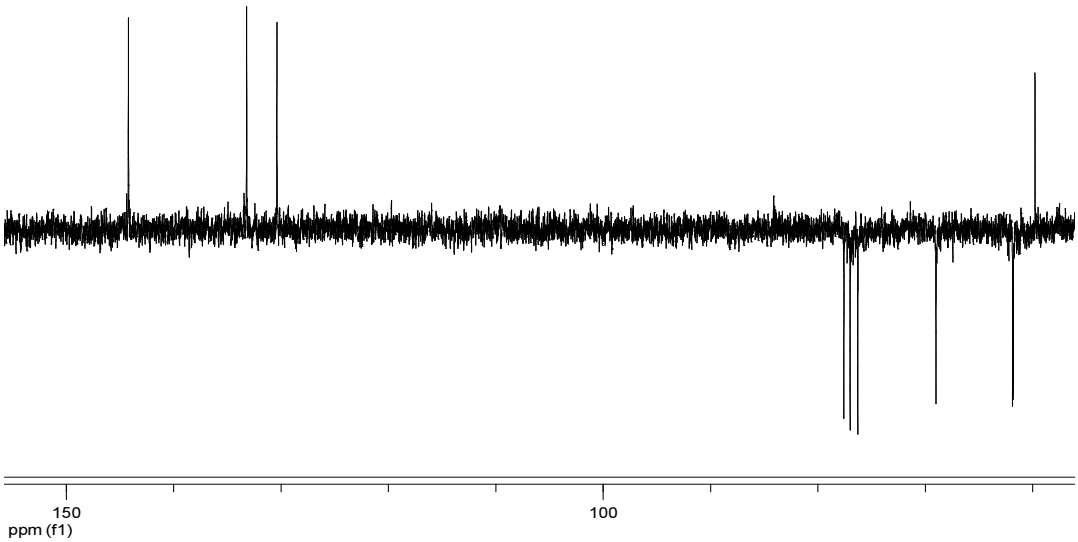
(4): ^{1}H-RMN ($CDCl_3$, 300 MHz) (δ / ppm)



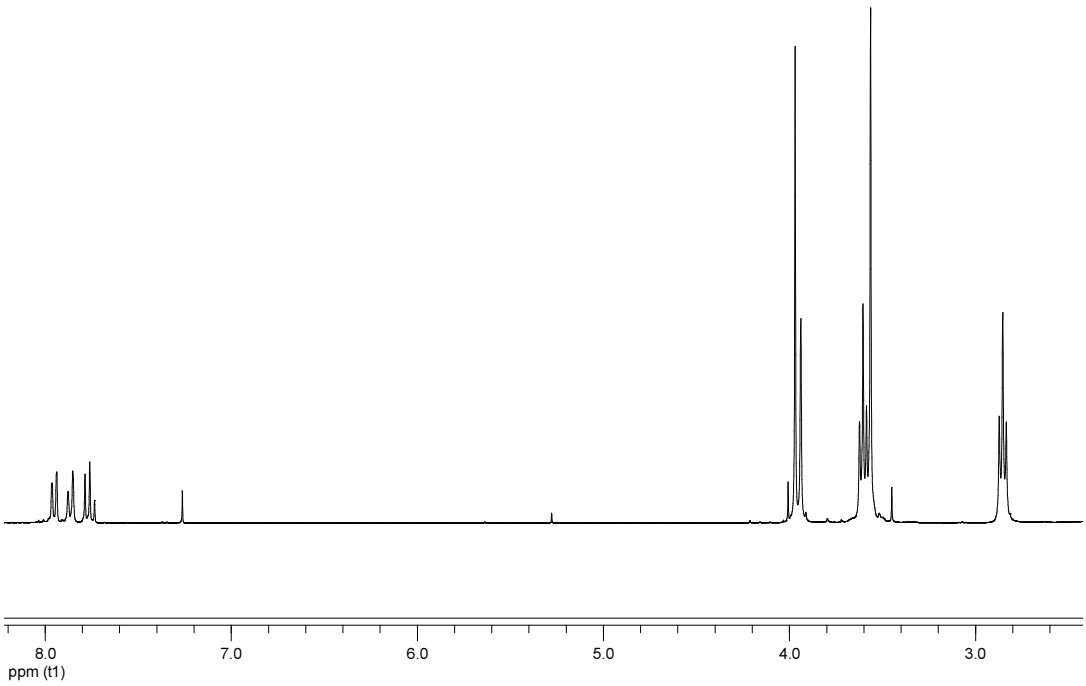
(4): ^{13}C-RMN ($CDCl_3$, 75.5 MHz) (δ / ppm)



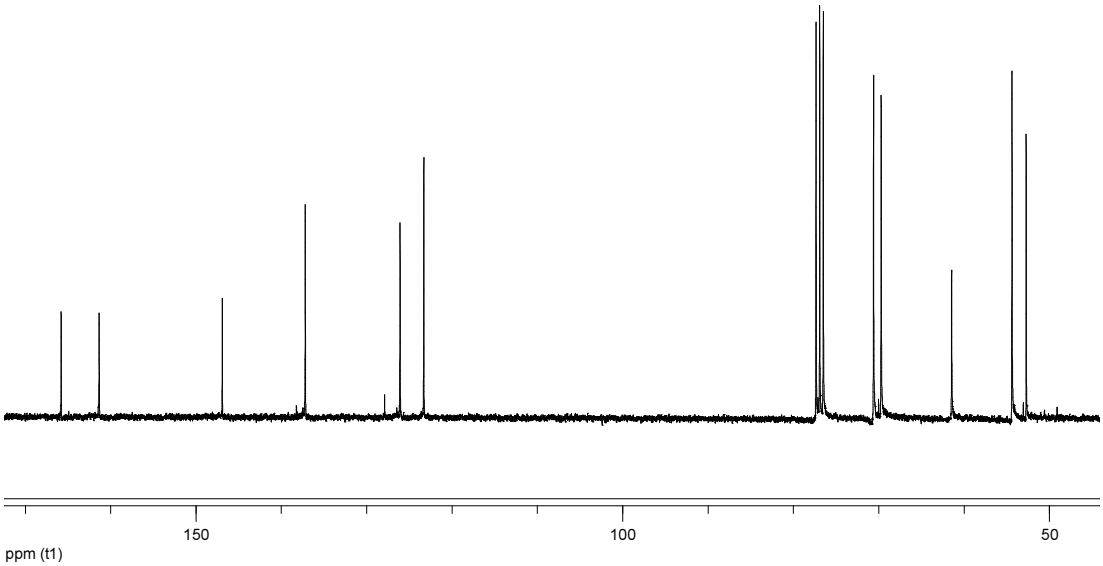
(4): ^{13}C- DEPT ($CDCl_3$, 75.5 MHz) (δ / ppm)



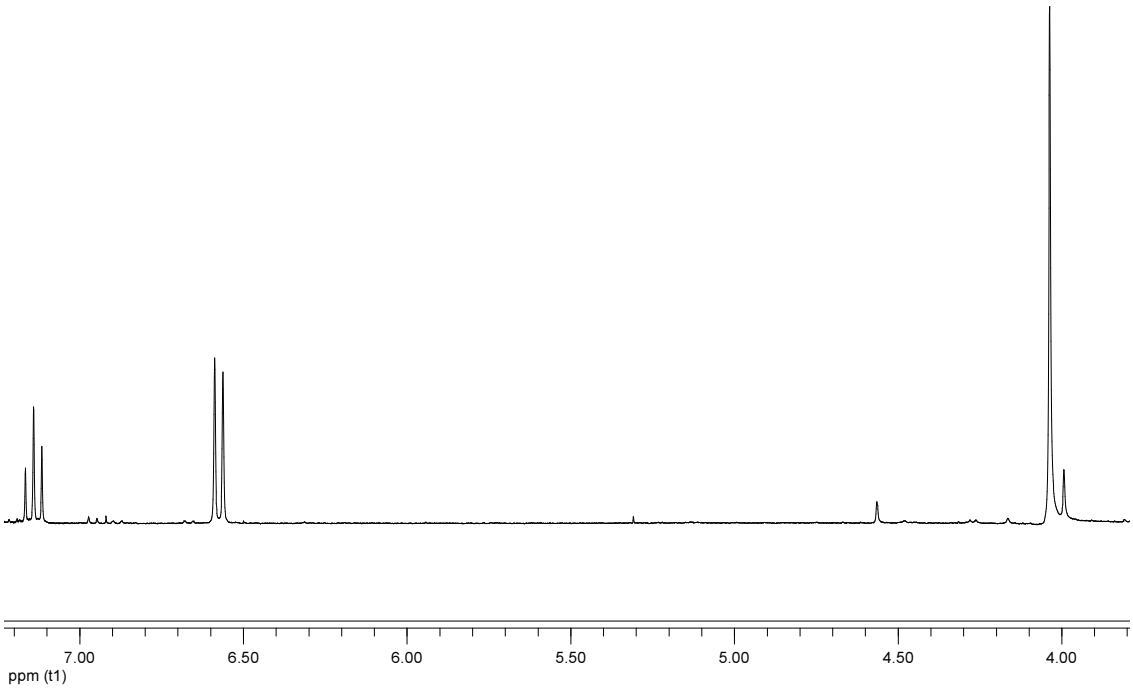
(6): ^{1}H-RMN ($CDCl_3$, 300 MHz) (δ / ppm)



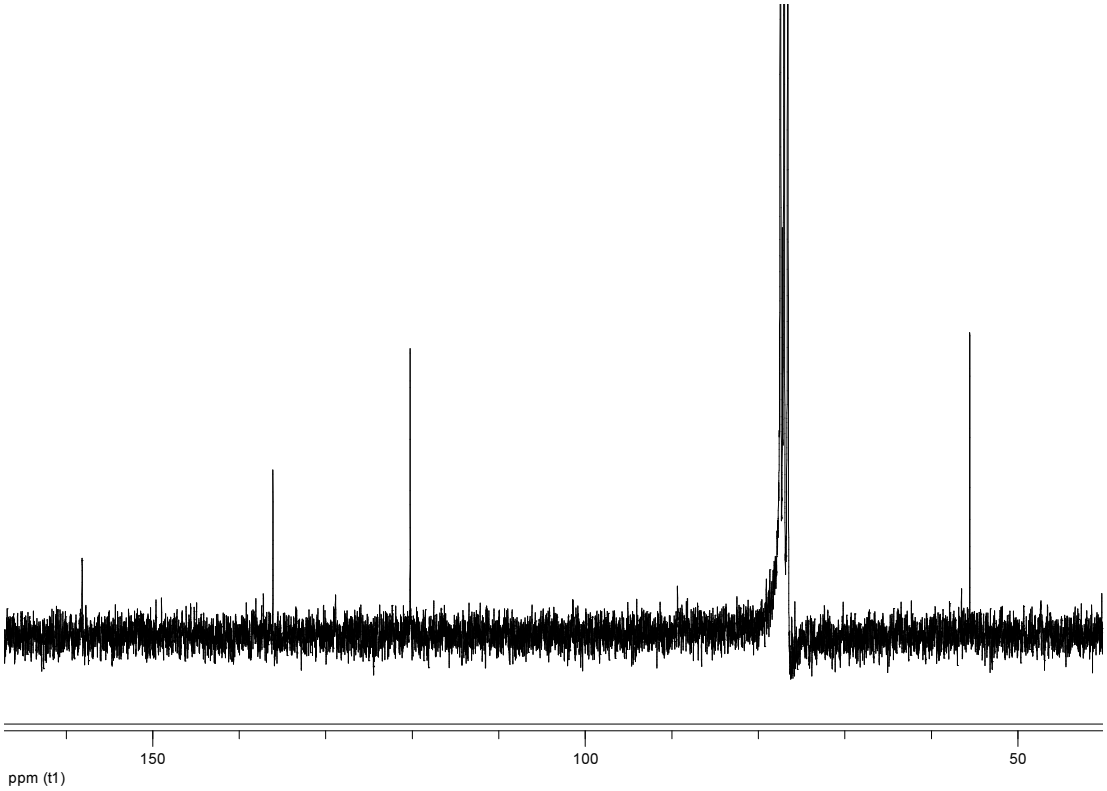
(6): ^{13}C-RMN ($CDCl_3$, 75.5 MHz) (δ / ppm)



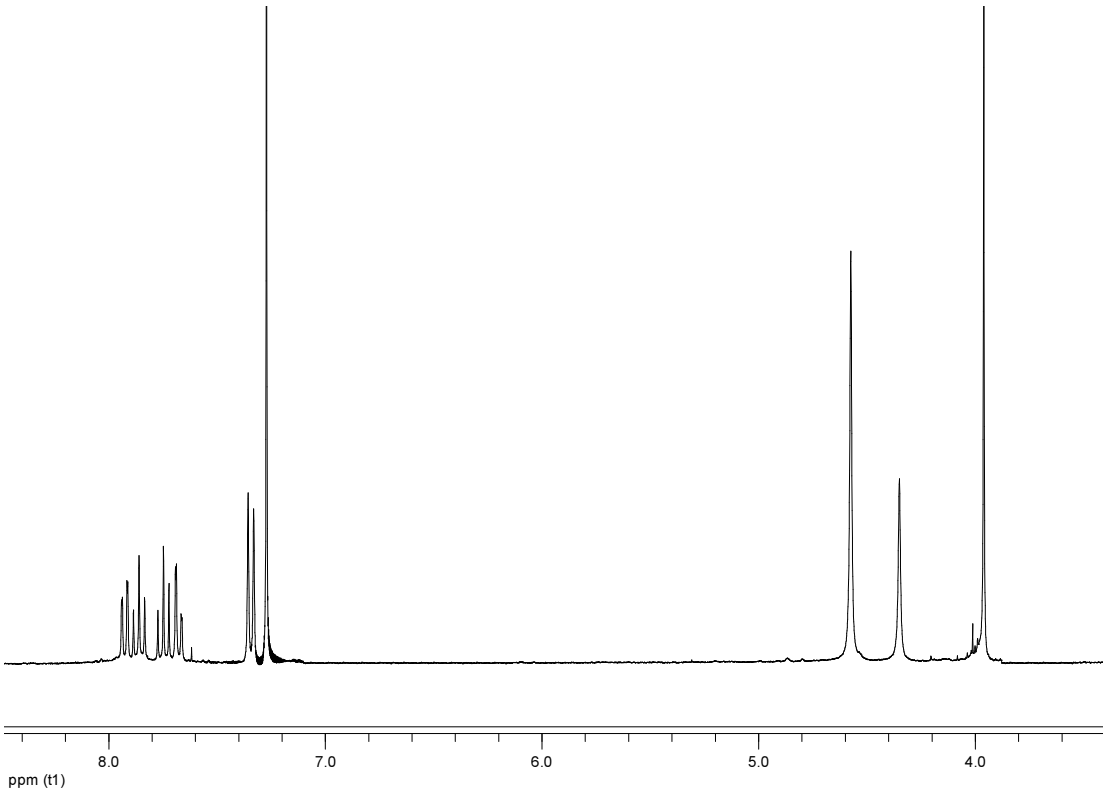
(7): ^{1}H-RMN ($CDCl_3$, 300 MHz) (δ / ppm)



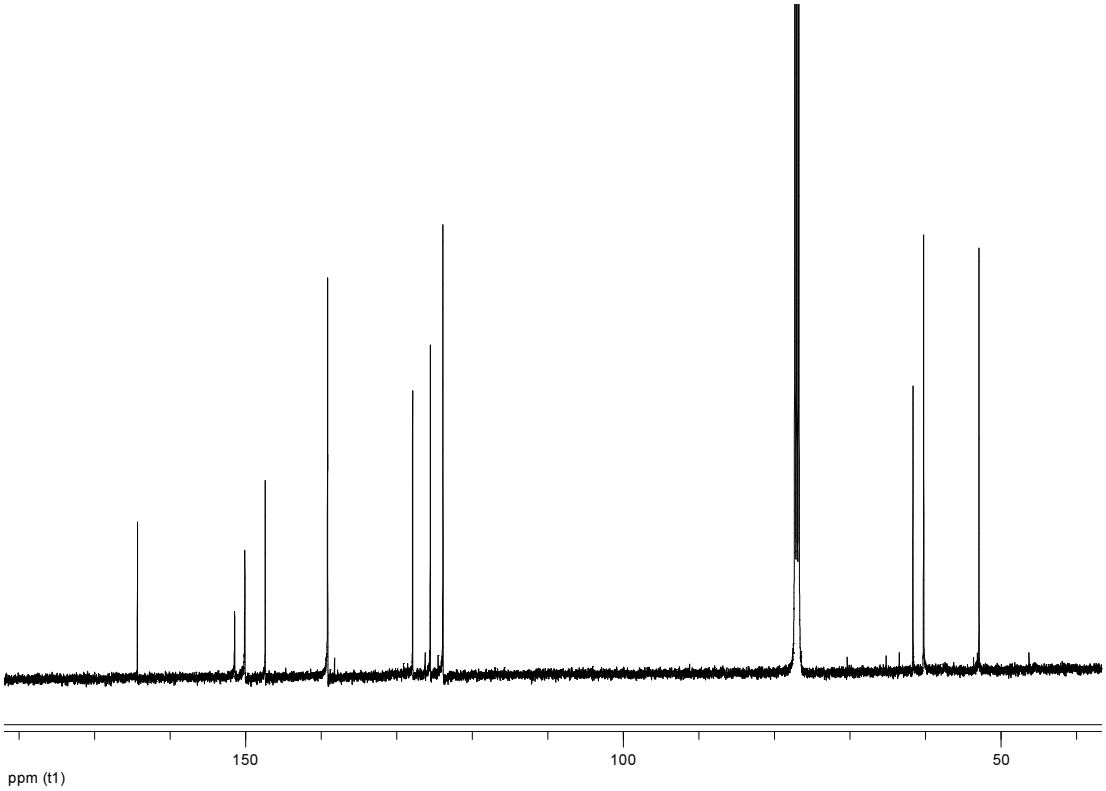
(7): ^{13}C-RMN ($CDCl_3$, 125.8 MHz) (δ / ppm)



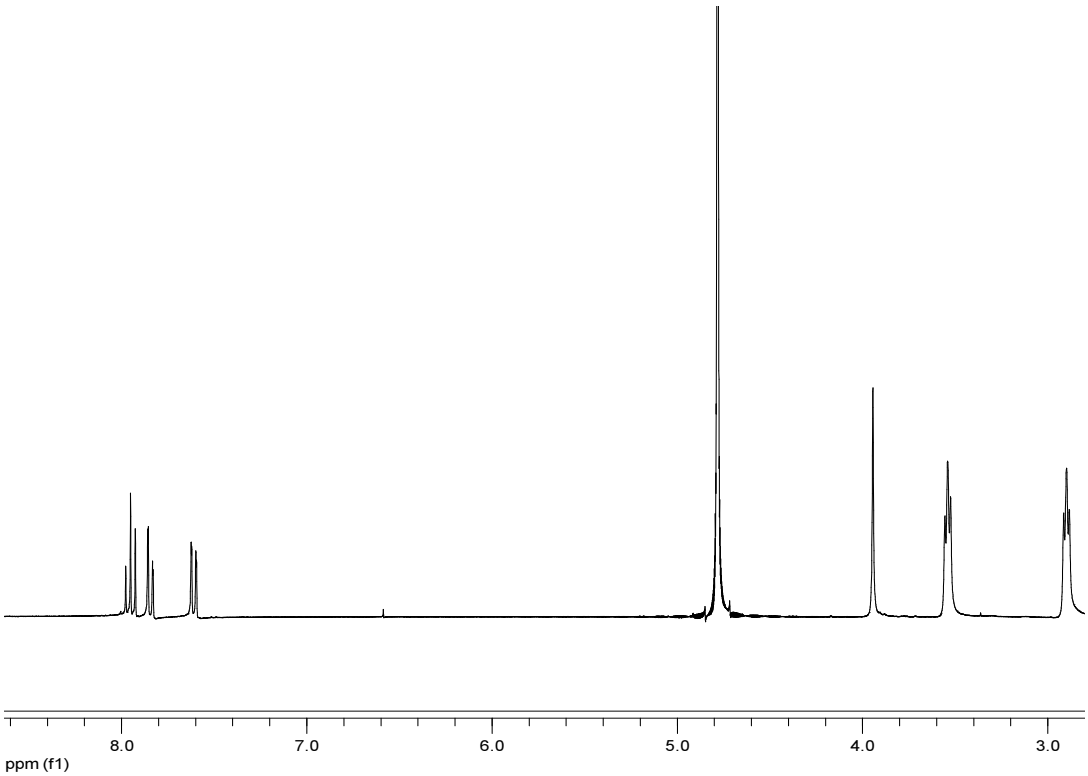
(9): ^{1}H-RMN ($CDCl_3$, 300 MHz) (δ / ppm)



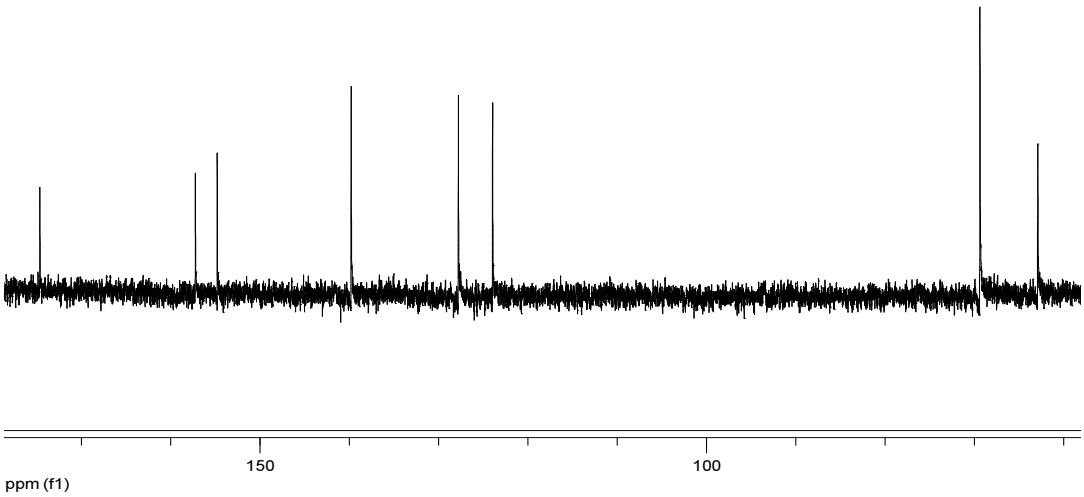
(9): ^{13}C-RMN ($CDCl_3$, 125.8 MHz) (δ / ppm)



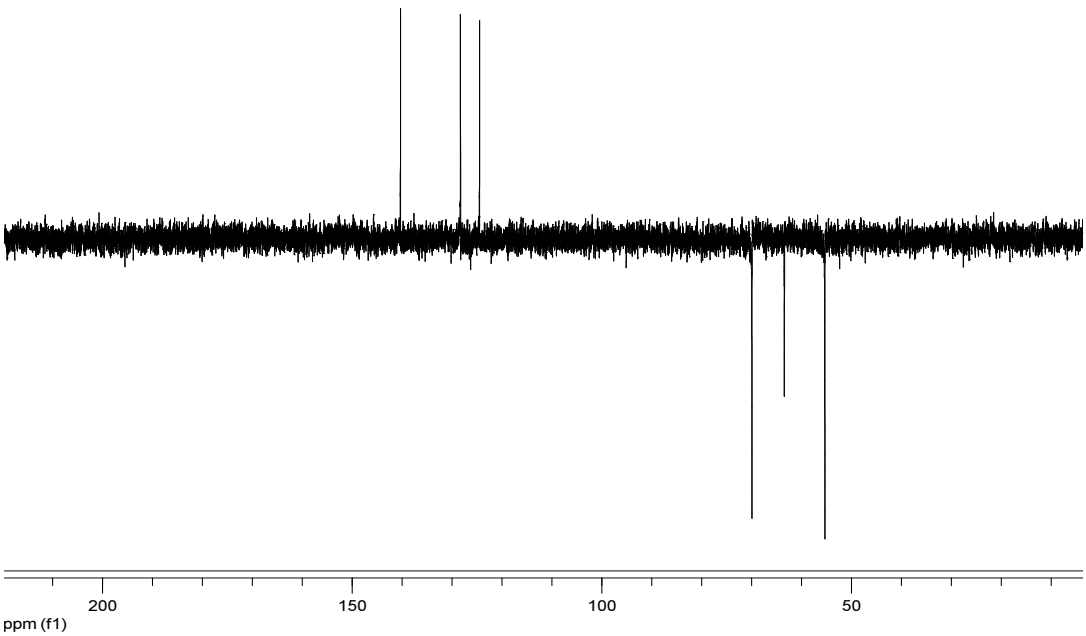
(H_2dpa12c4): ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



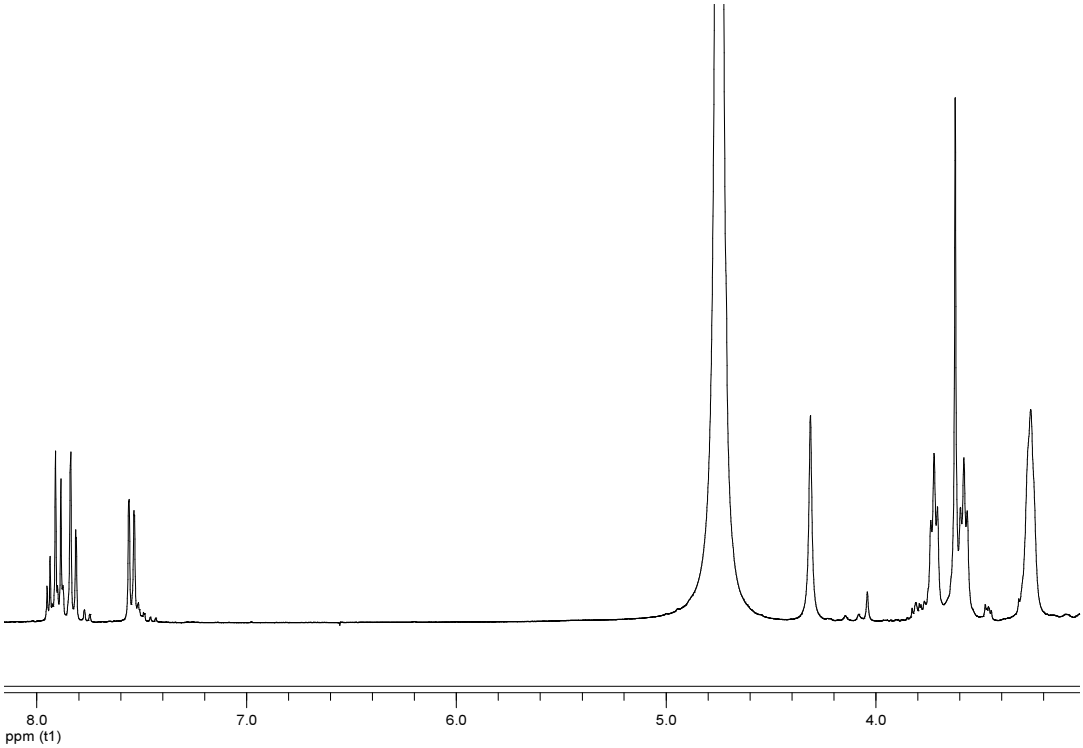
(H_2dpa12c4): ^{13}C-RMN (D_2O, 75.5 MHz) (δ / ppm)



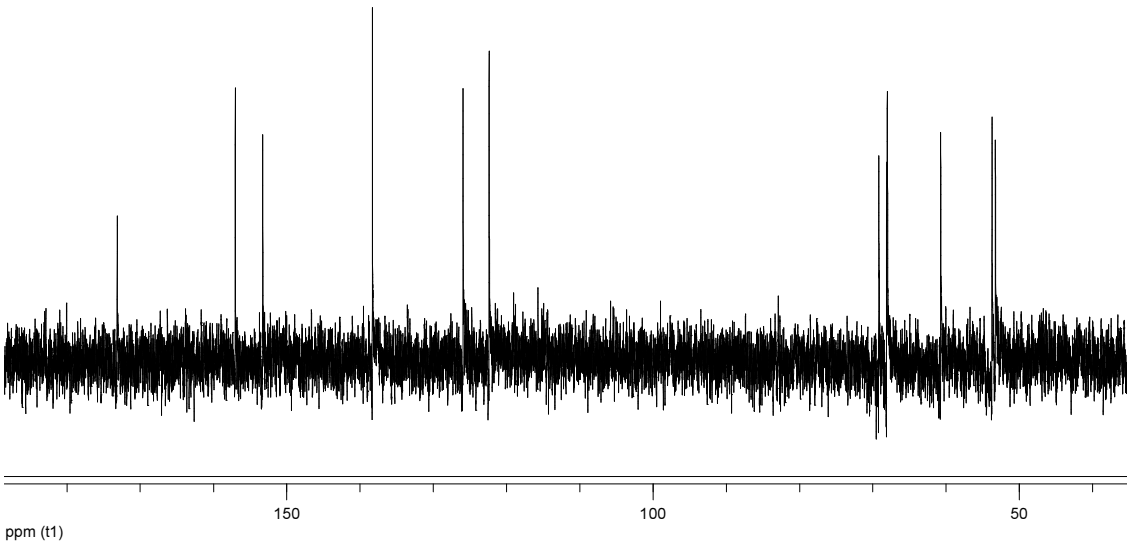
(H_2dpa12c4): ^{13}C- DEPT (D_2O, 75.5 MHz) (δ / ppm)



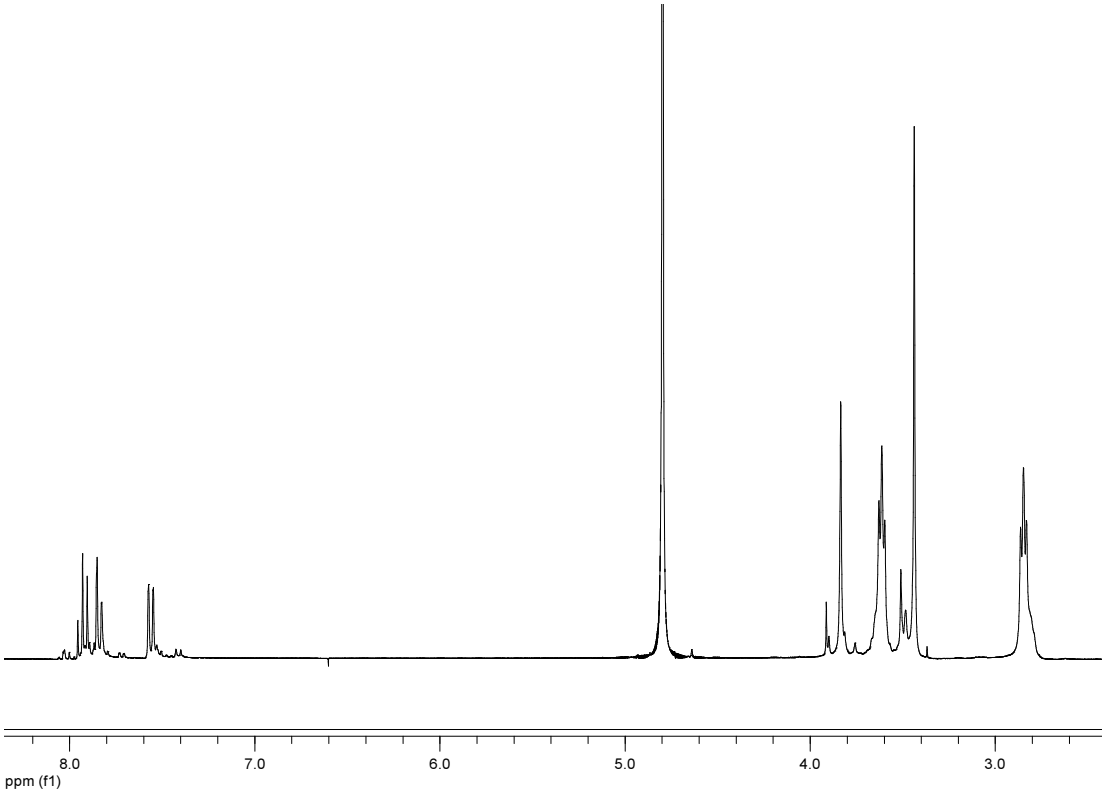
(H_2dpa15c5): ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



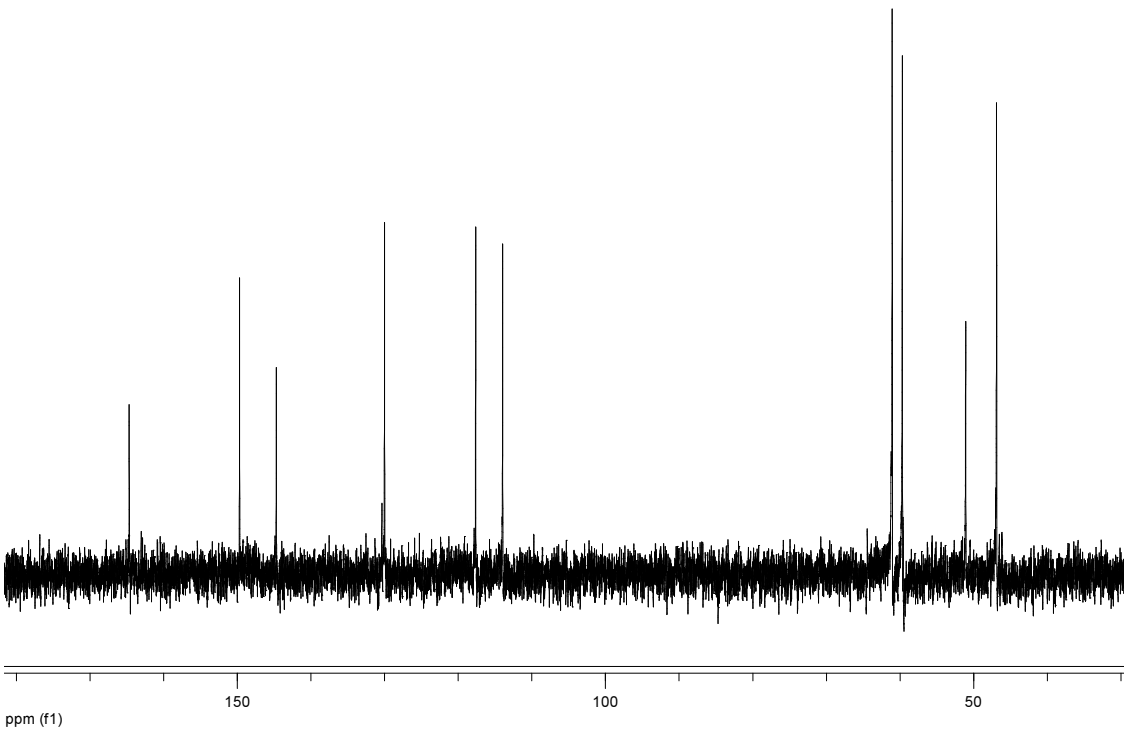
(H_2dpa15c5): ^{13}C-RMN (D_2O, 75.5 MHz) (δ / ppm)



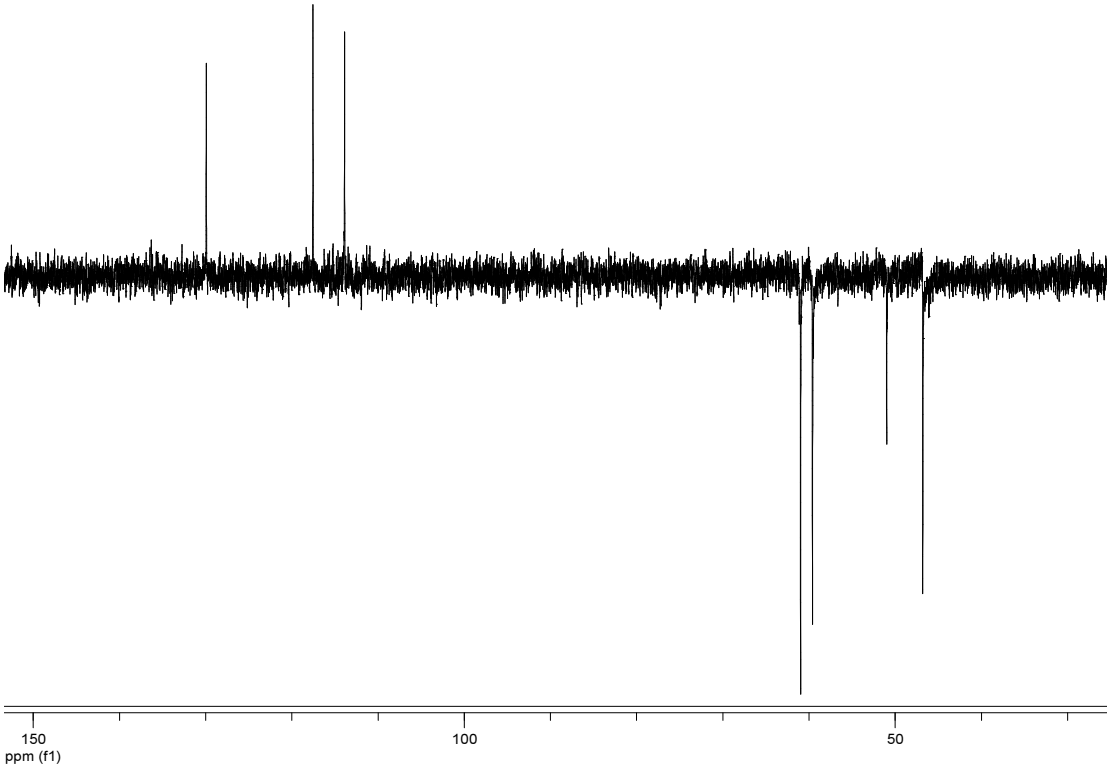
(H_2dpa18c6): ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



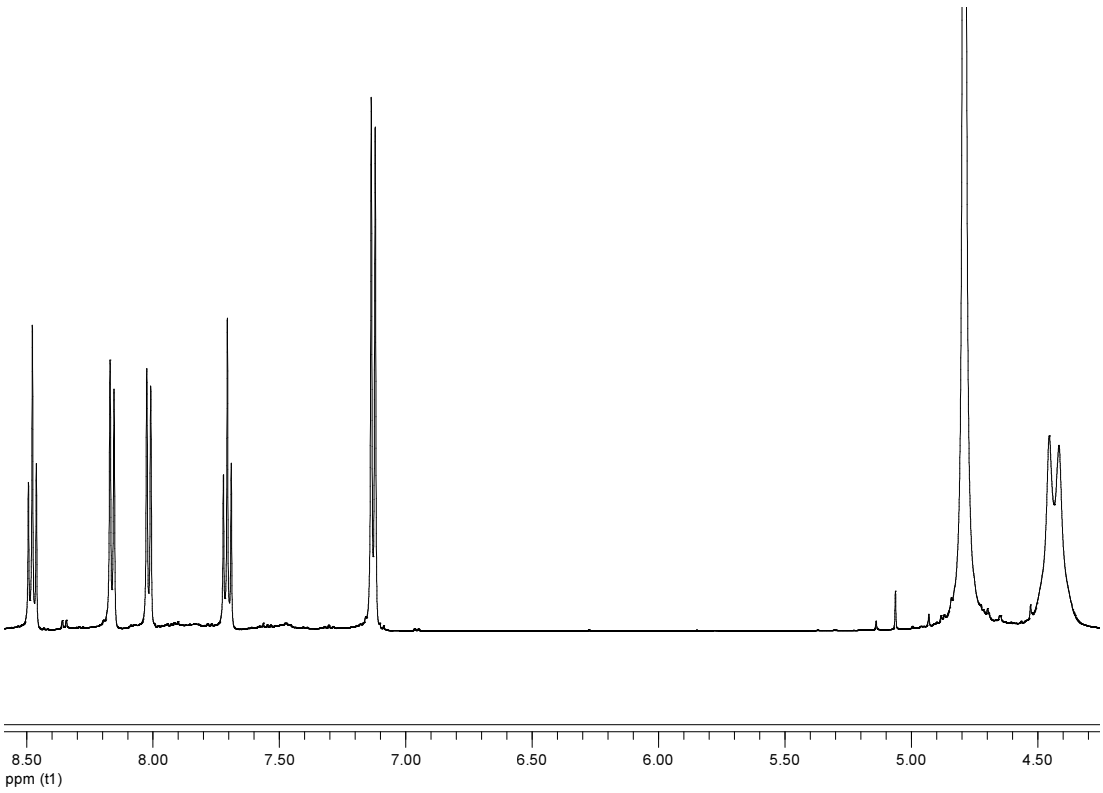
(H_2dpa18c6): ^{13}C-RMN (D_2O, 75.5 MHz) (δ / ppm)



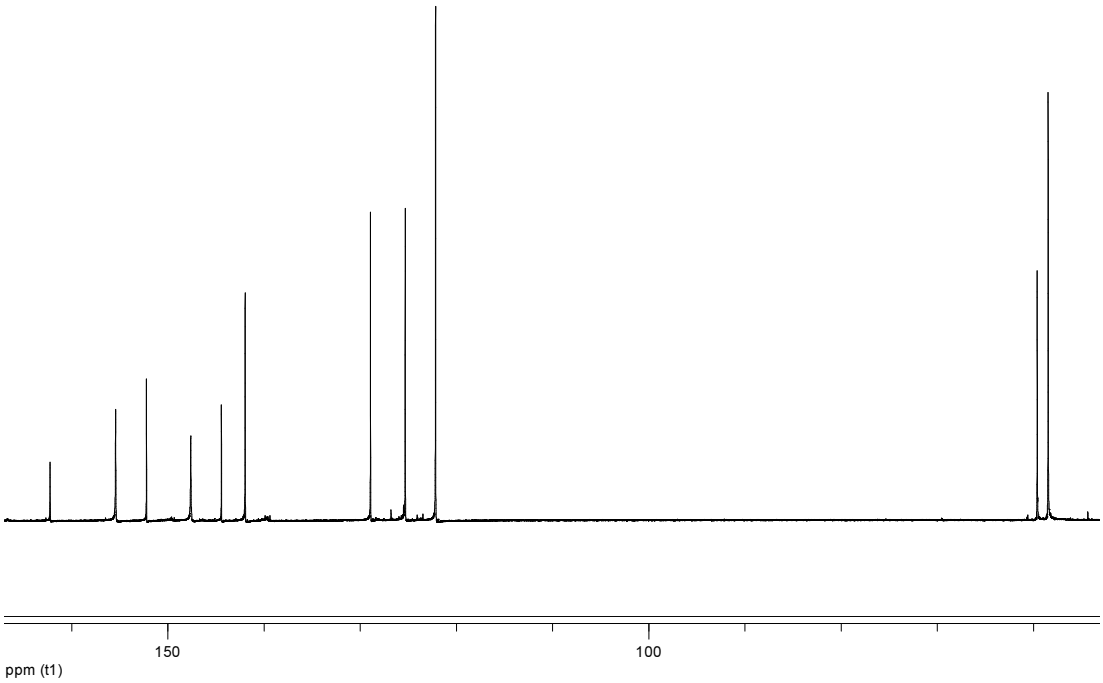
(H_2dpa18c6): ^{13}C- DEPT(D_2O, 75.5 MHz) (δ / ppm)



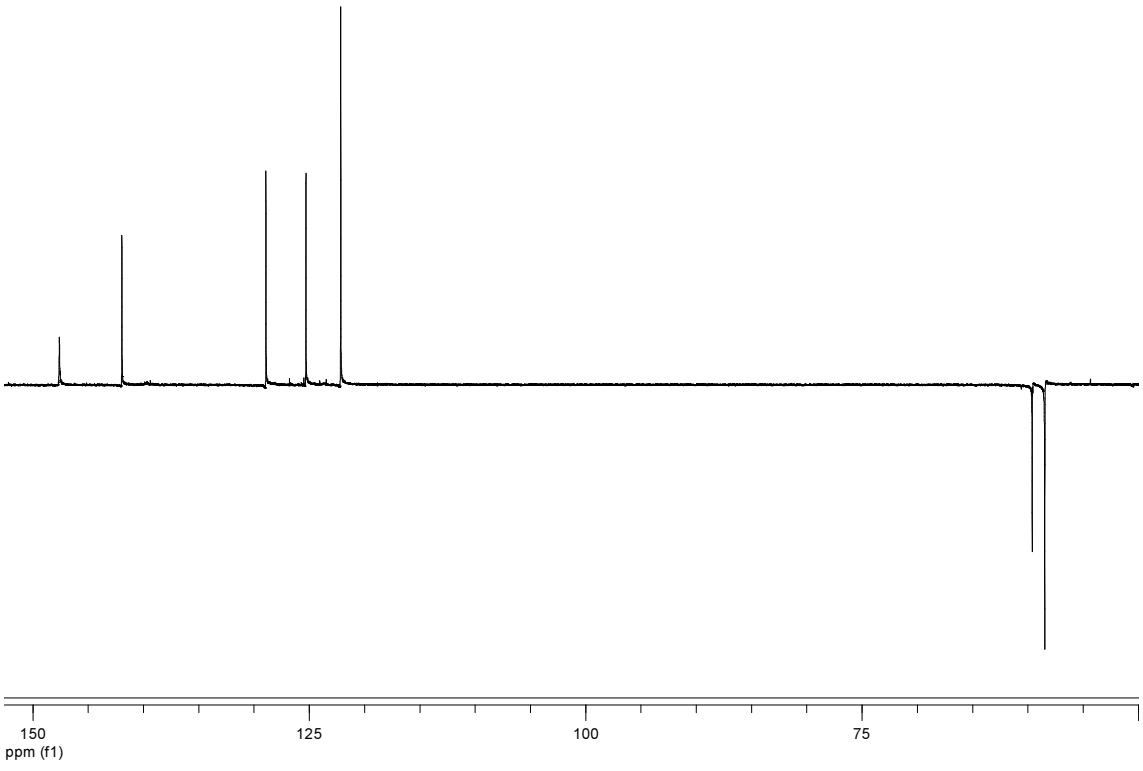
(H_2dpabp): ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



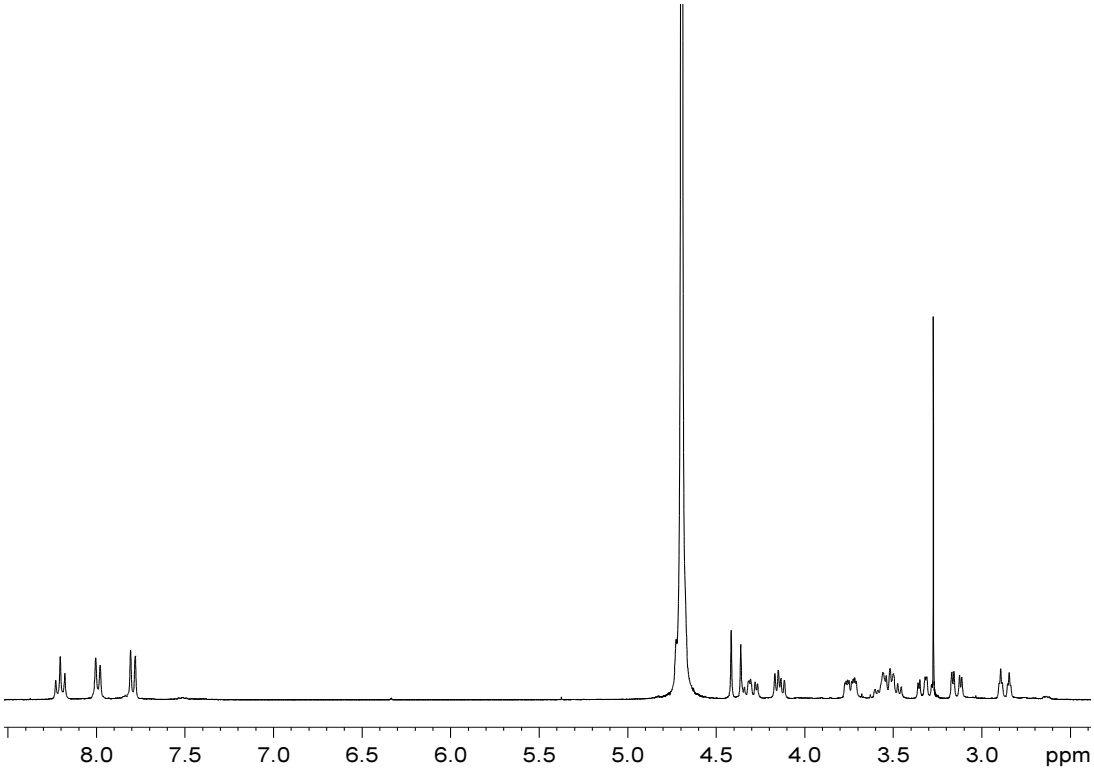
(H_2dpabp): ^{13}C-RMN (D_2O, 125.8 MHz) (δ / ppm)



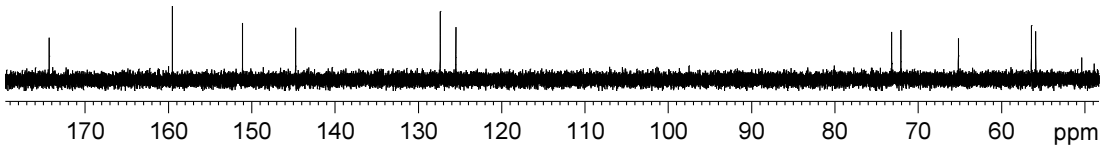
(H_2dpabp): ^{13}C- DEPT(D_2O, 128.5 MHz) (δ / ppm)



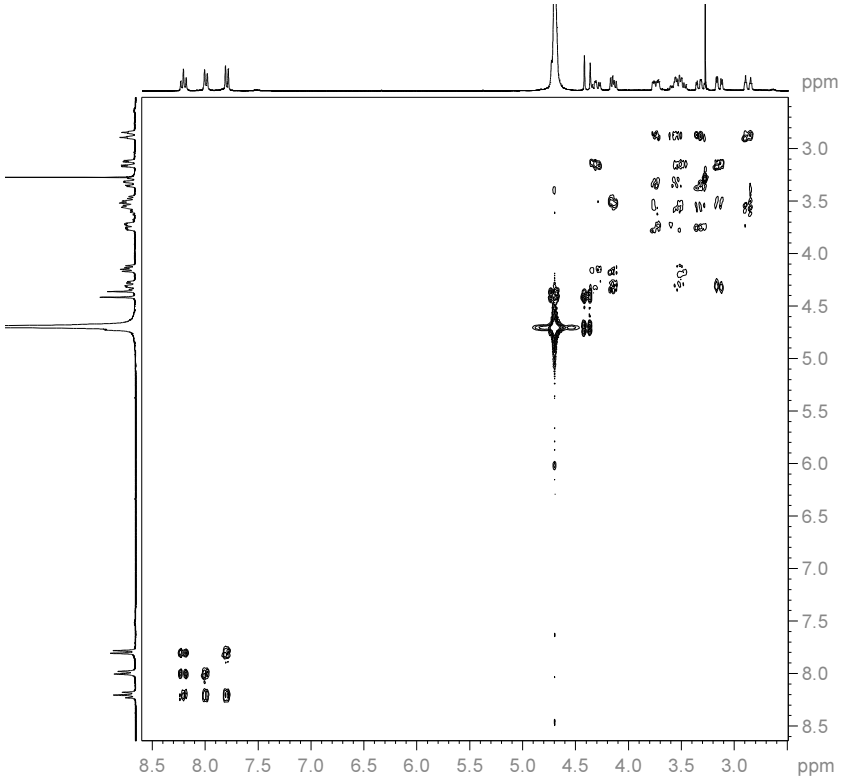
[Lu(dpa12c4)(H_2O)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



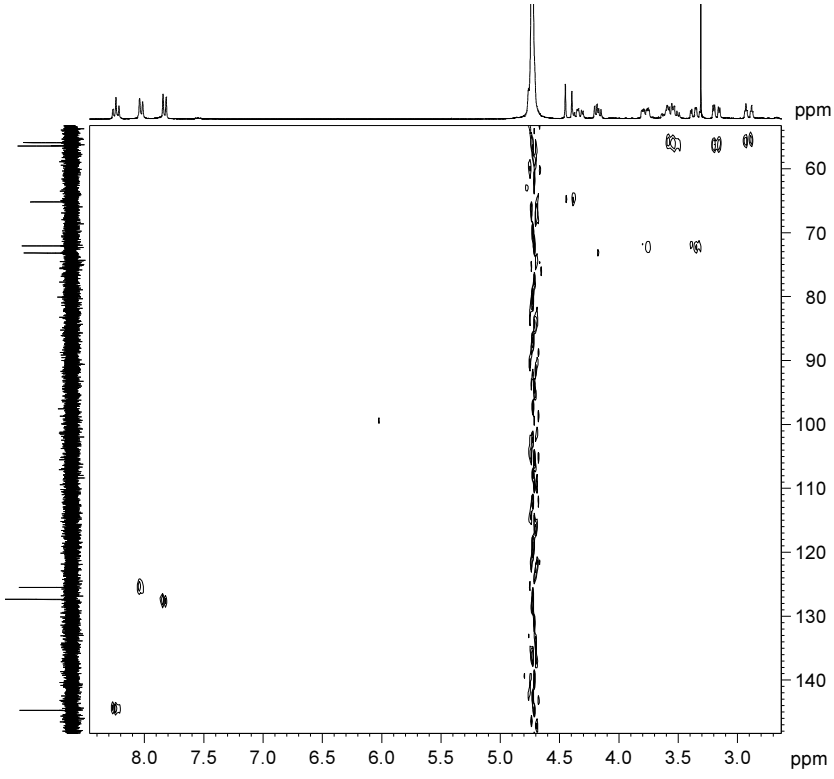
[Lu(dpa12c4)(H_2O)]: ^{13}C-RMN (D_2O, 75.5 MHz) (δ / ppm)



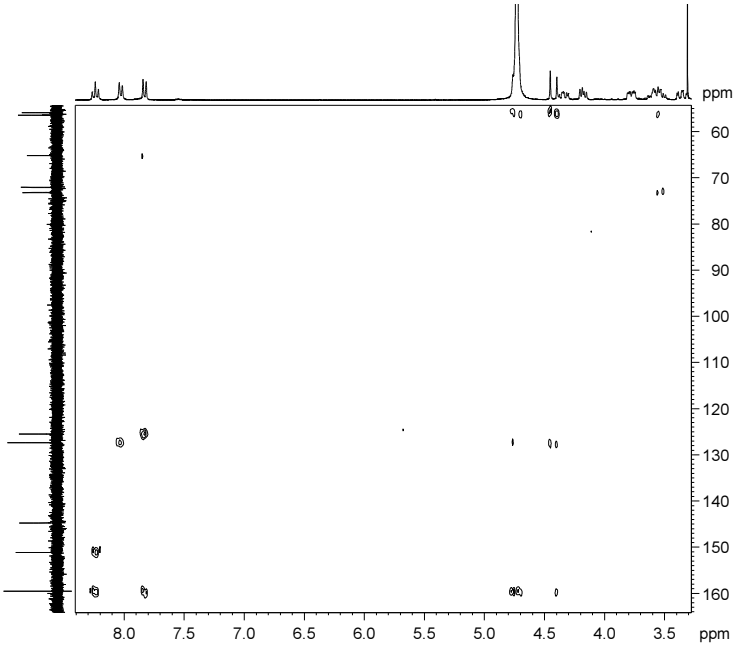
[Lu(dpa12c4)(H_2O)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



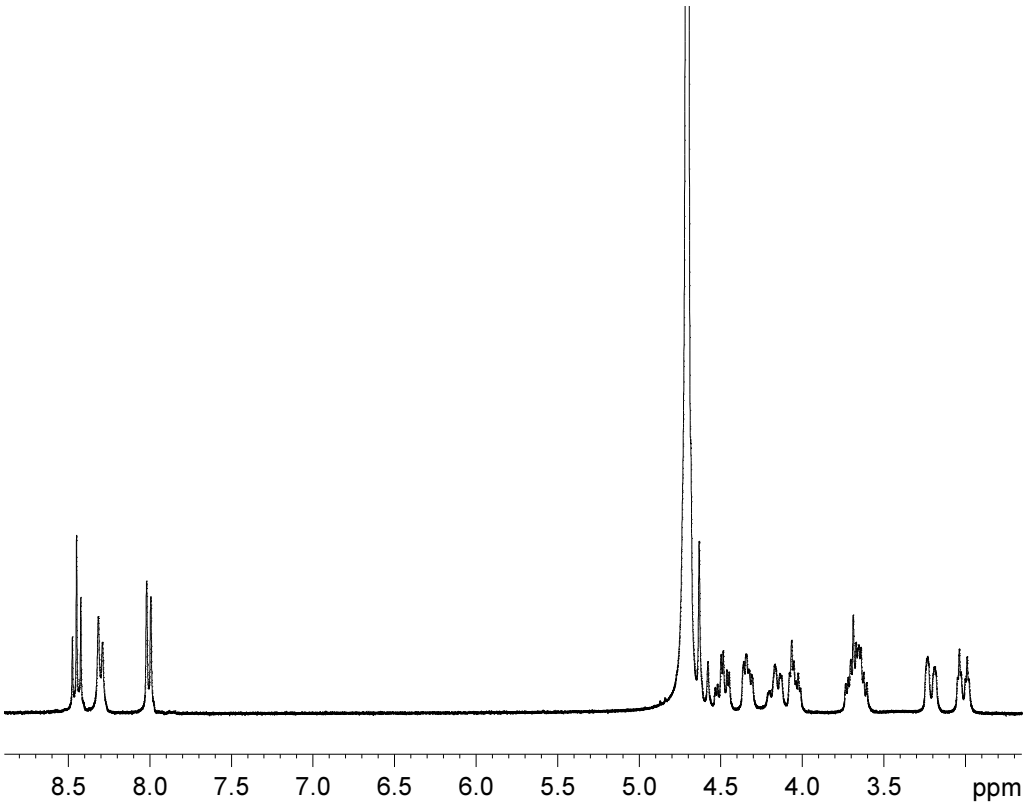
[Lu(dpa12c4)(H_2O)]: HSQC (D_2O, 300 MHz) (δ / ppm)



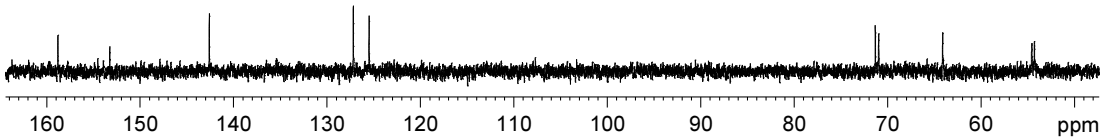
[Lu(dpa12c4)(H_2O)]: HMBC (D_2O, 300 MHz) (δ / ppm)



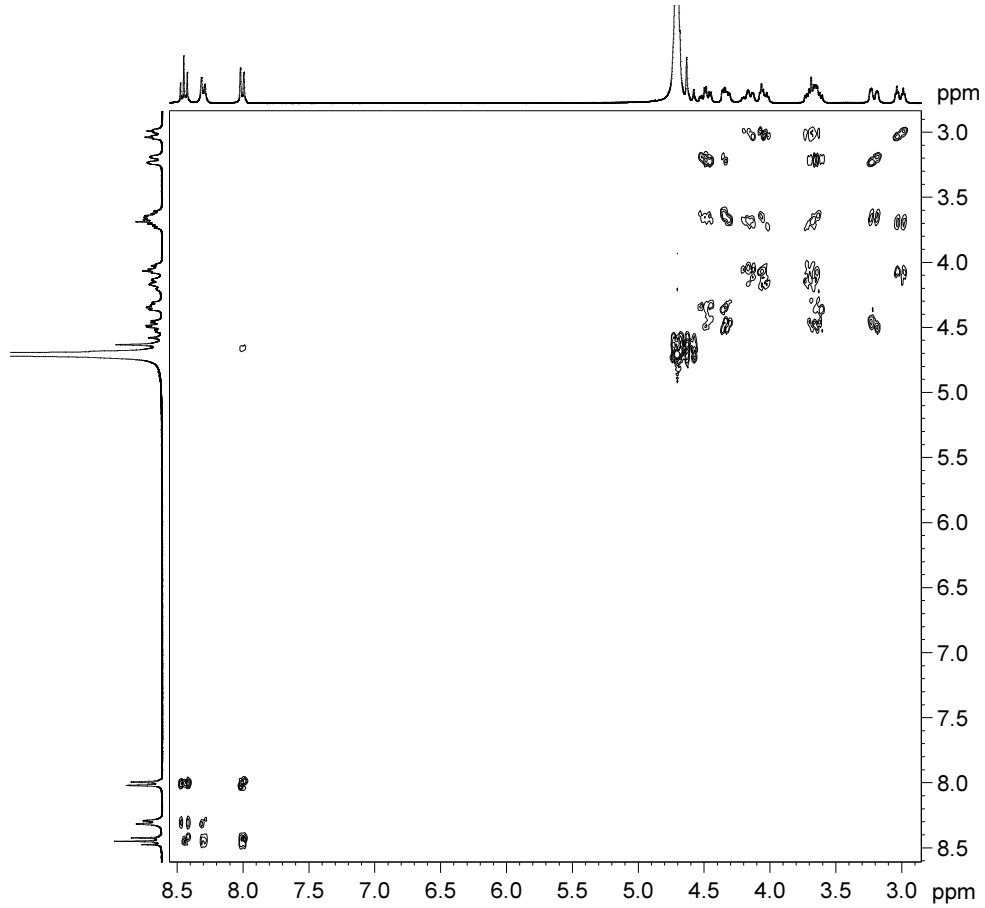
[La(dpa12c4)(H_2O)$_2$]: ^{1}H-RMN (D_2O, 300 MHz, 348 K) (δ / ppm)



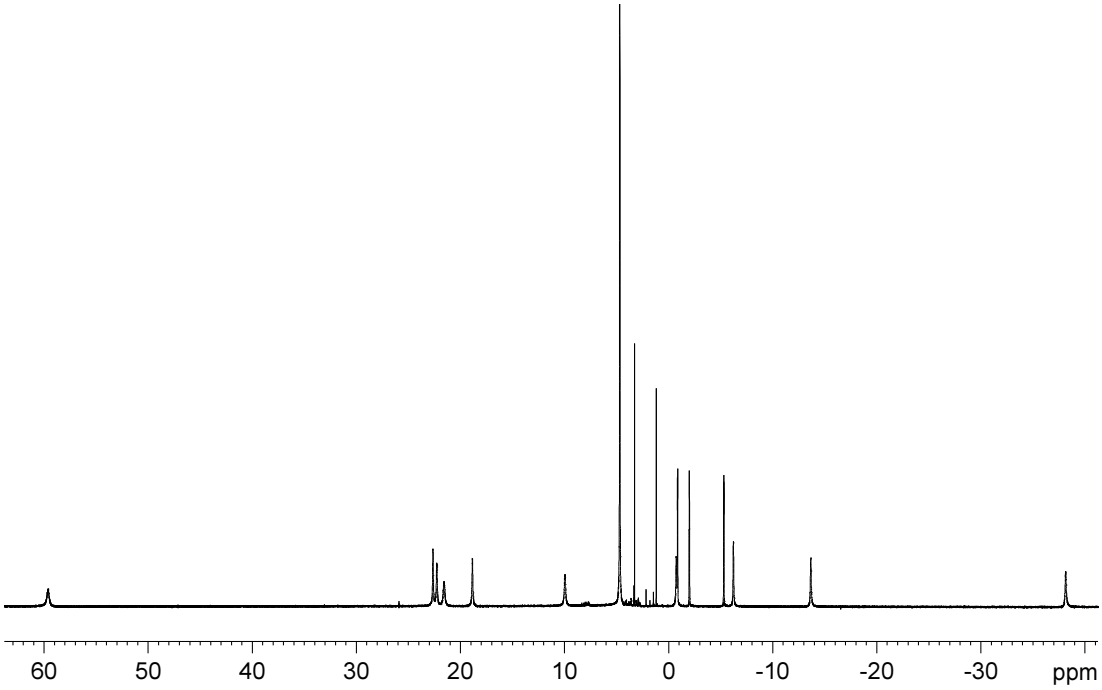
[La(dpa12c4)(H_2O)$_2$]: ^{13}C-RMN (D_2O, 75.5 MHz, 348 K) (δ / ppm)



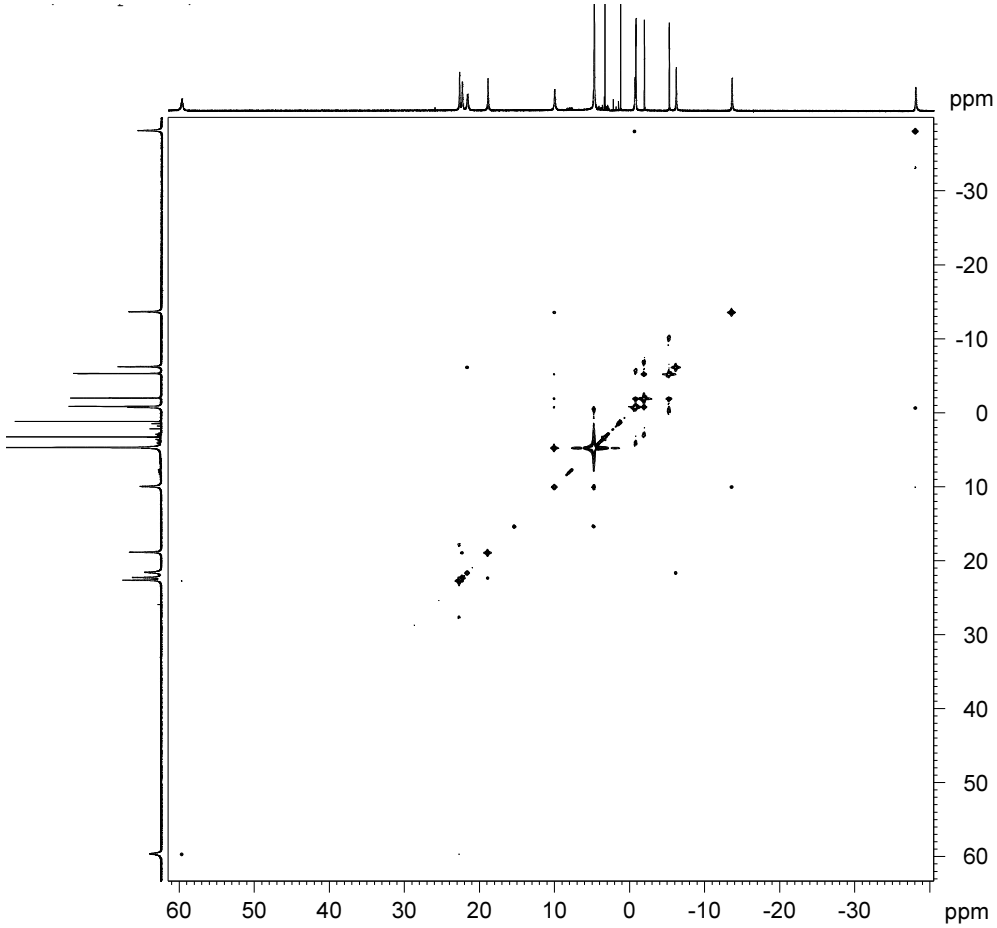
[La(dpa12c4)(H_2O)$_2$]: ^{1}H-COSY (D_2O, 300 MHz, 348 K) (δ / ppm)



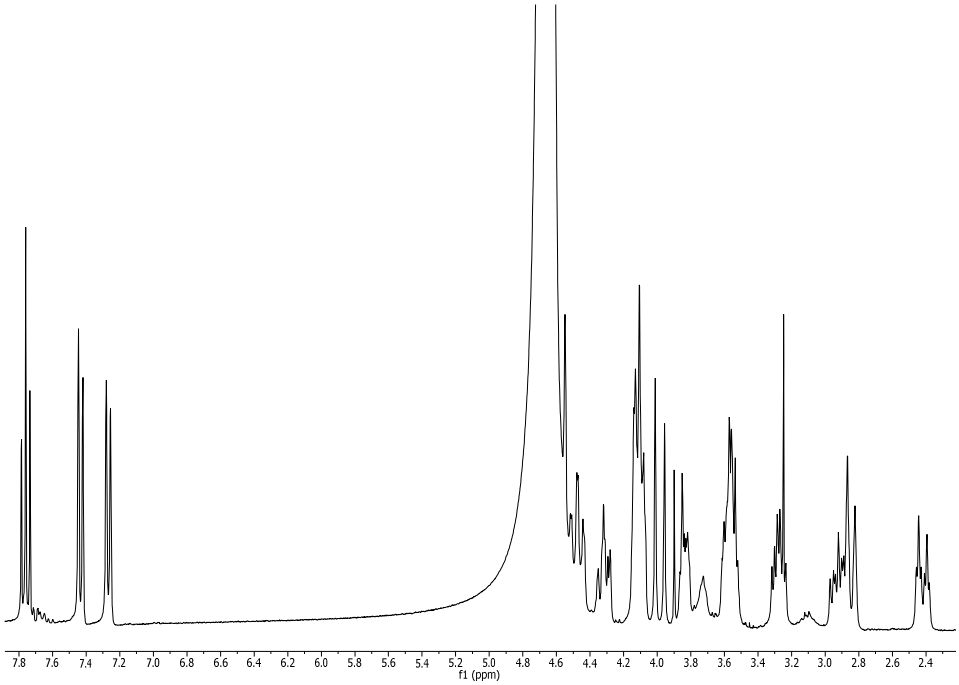
[Yb(bp12c4)(H_2O)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



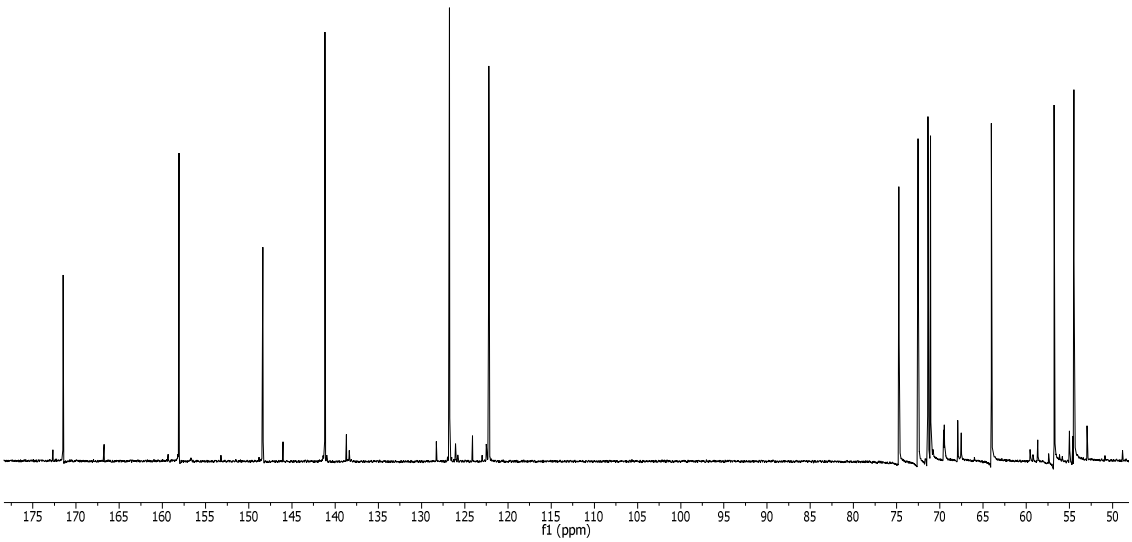
[Yb(dpa12c4)(H_2O)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



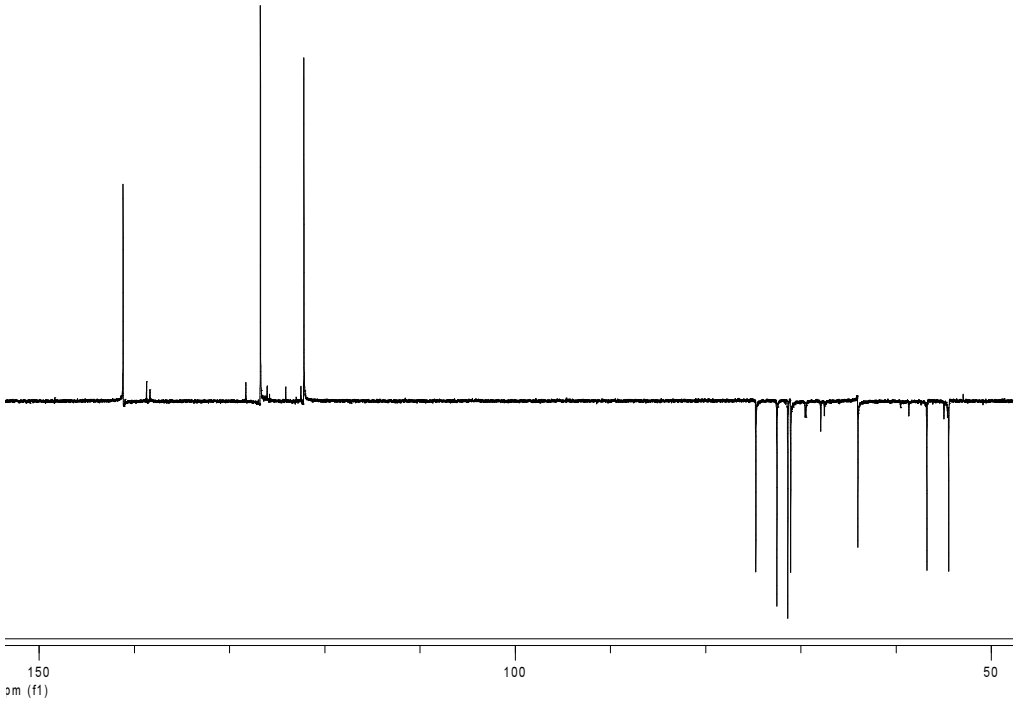
[Lu(dpa18c6)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



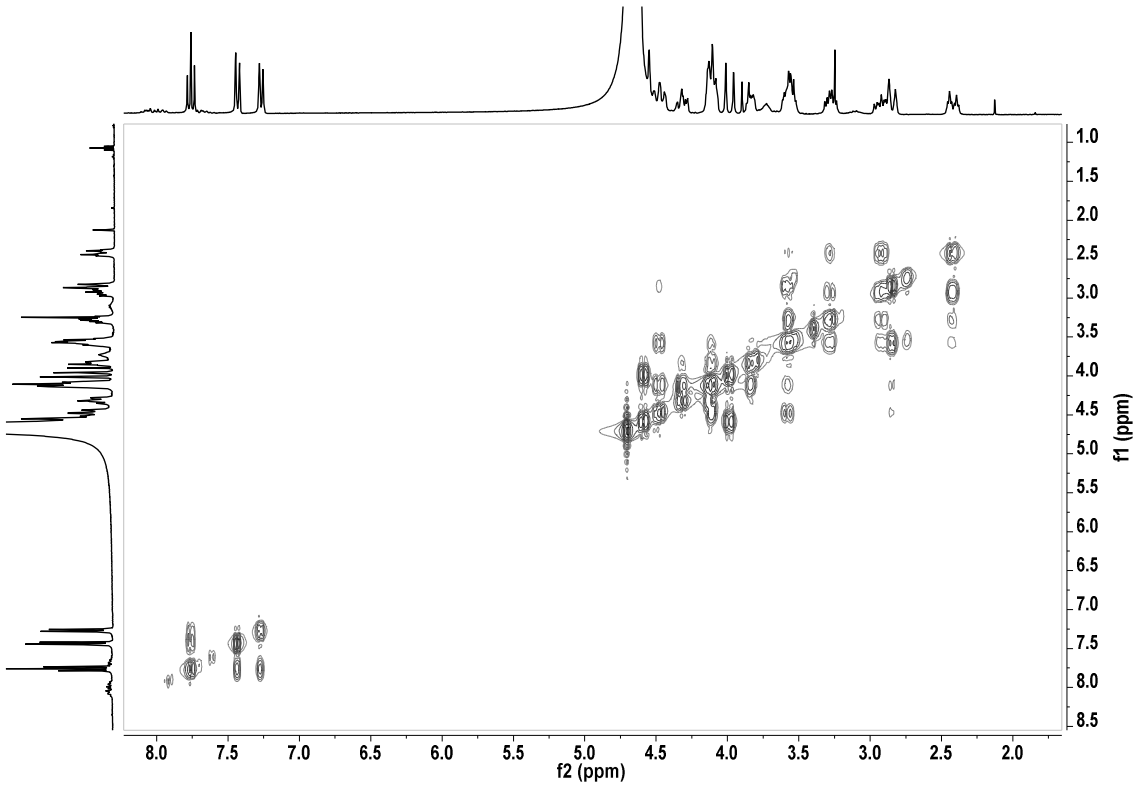
[Lu(dpa18c6)]: ^{13}C-RMN (D_2O, 125.8 MHz) (δ / ppm)



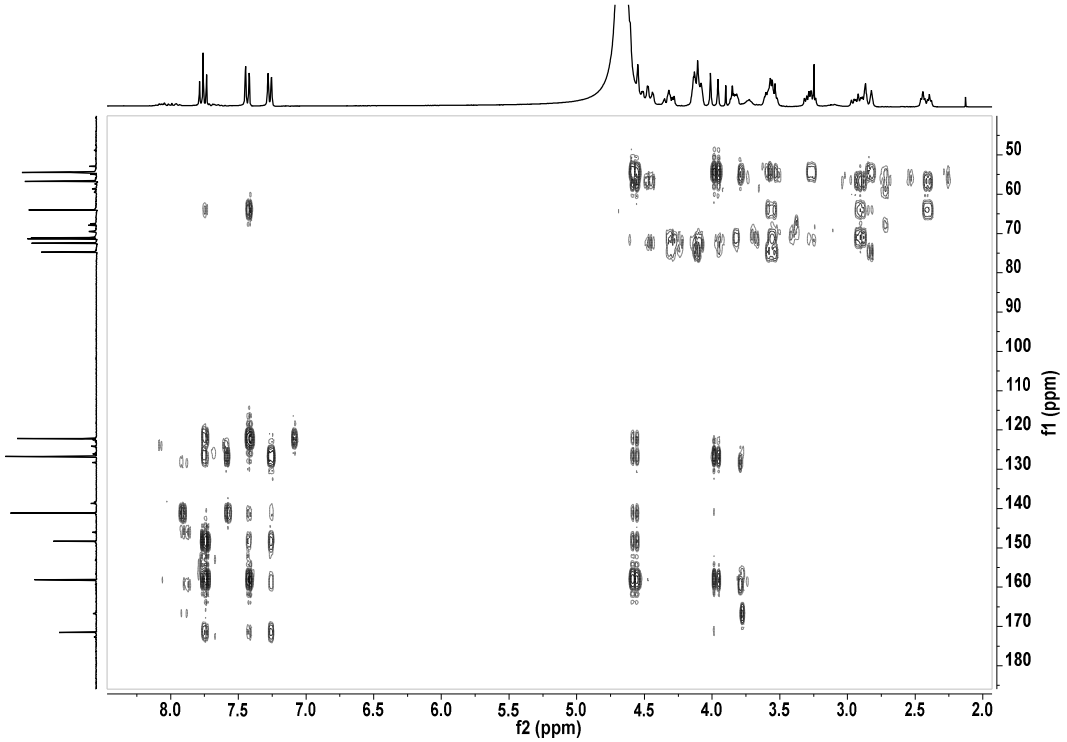
[Lu(dpa18c6)]: ^{13}C-DEPT (D_2O, 125.8 MHz) (δ / ppm)



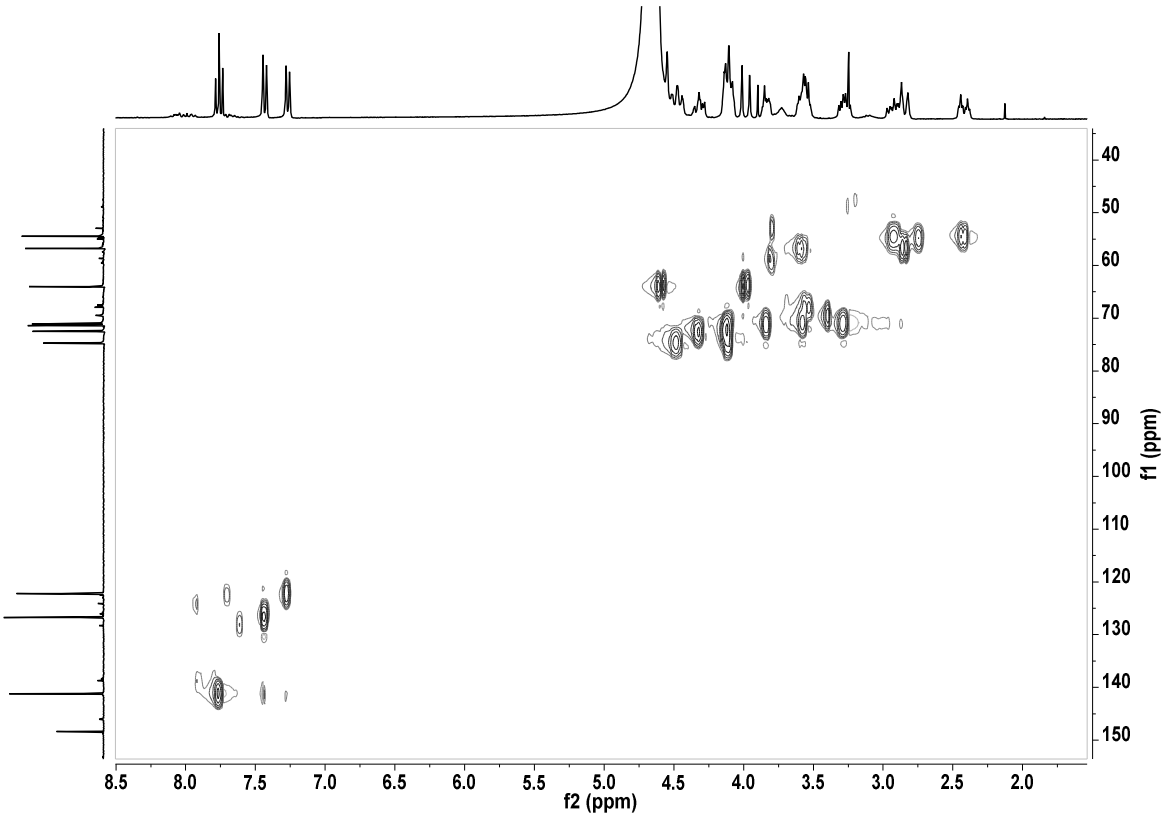
[Lu(dpa18c6)]: ^{1}H-COSY (D_2O, 500 MHz) (δ / ppm)



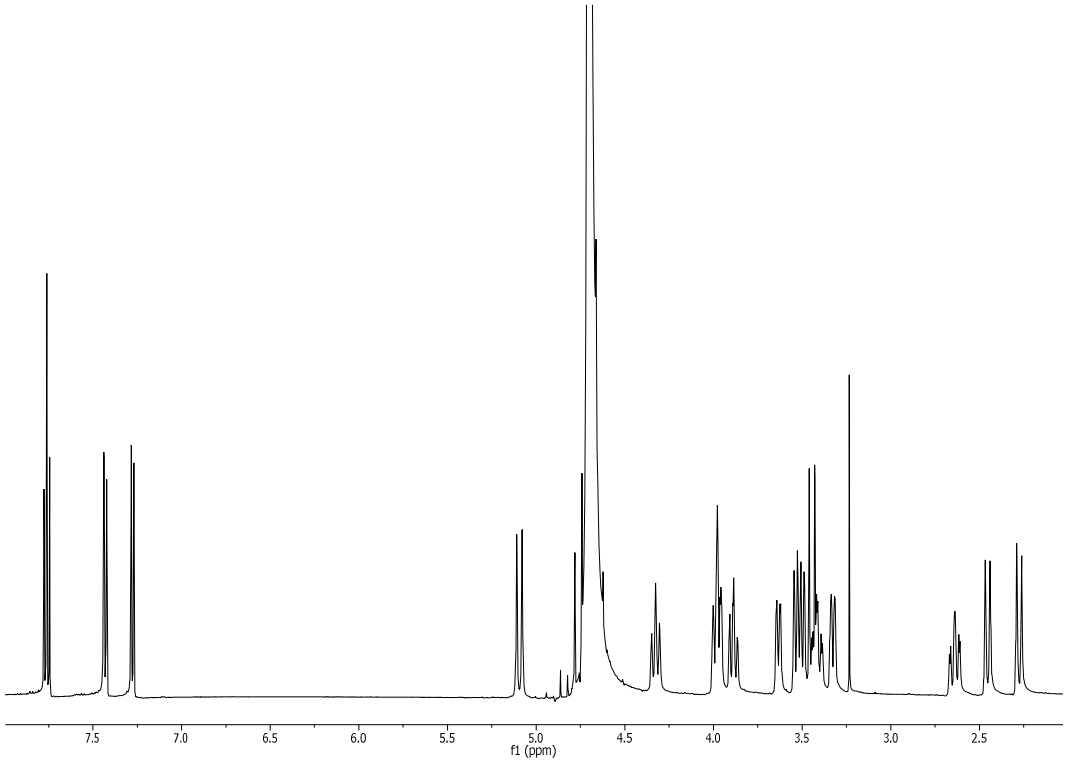
[Lu(dpa18c6)]: ^{1}H-HMBC (D_2O, 500 MHz) (δ / ppm)



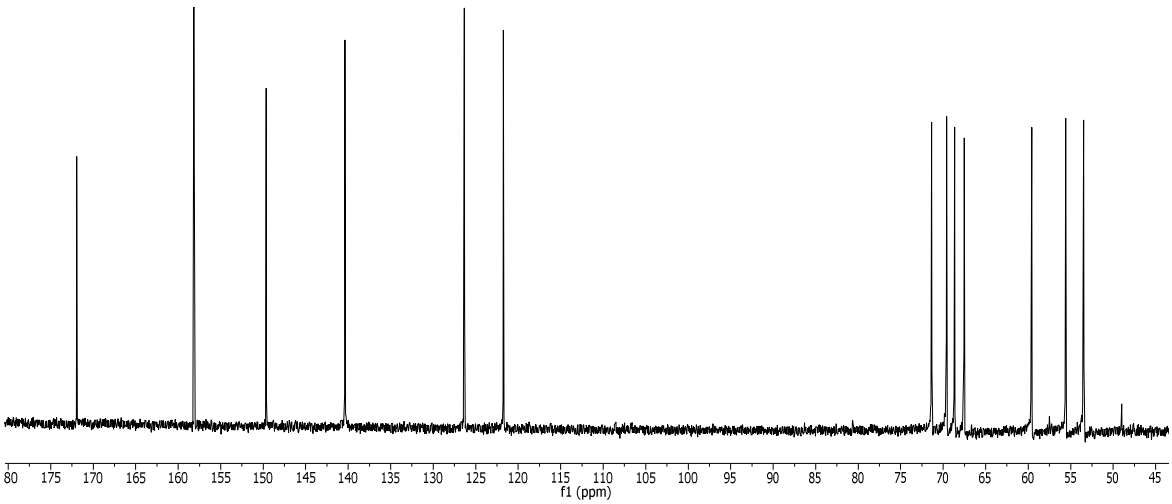
[Lu(dpa18c6)]: ^{1}H-HSQC (D_2O, 500 MHz) (δ / ppm)



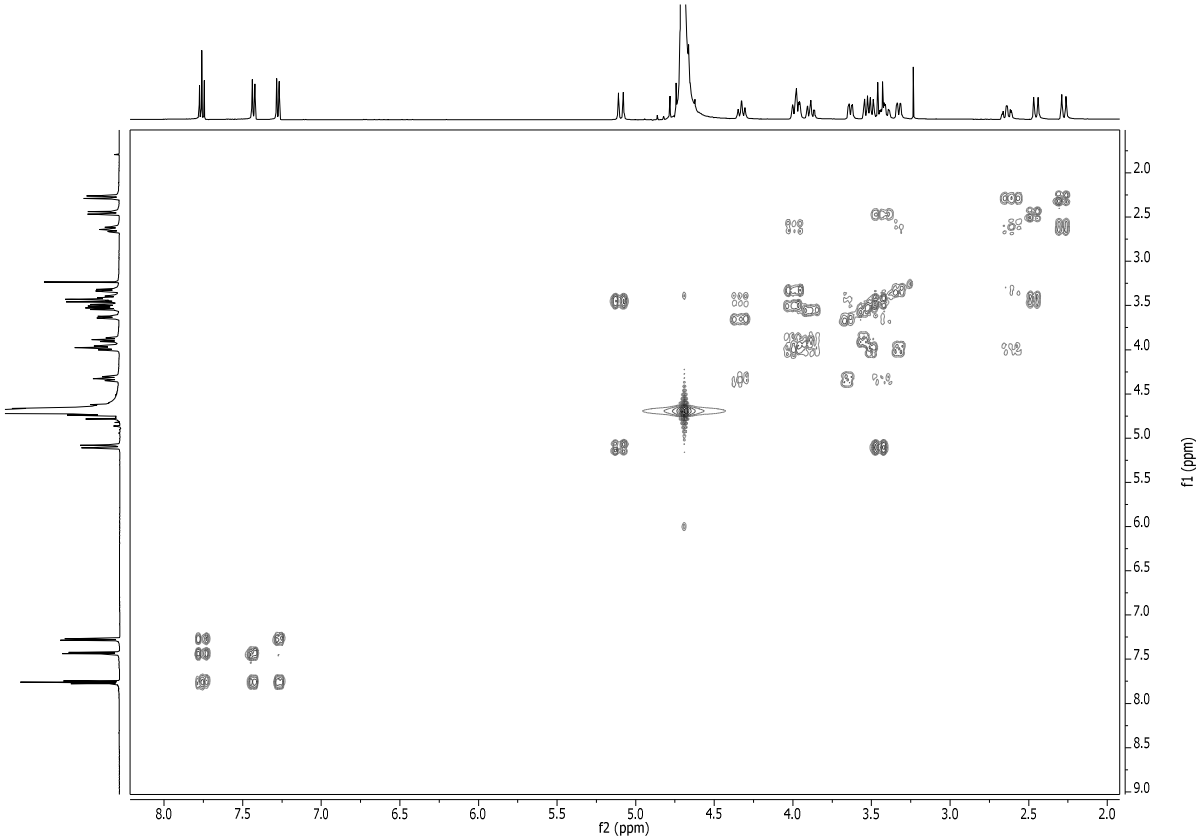
[La(dpa18c6)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



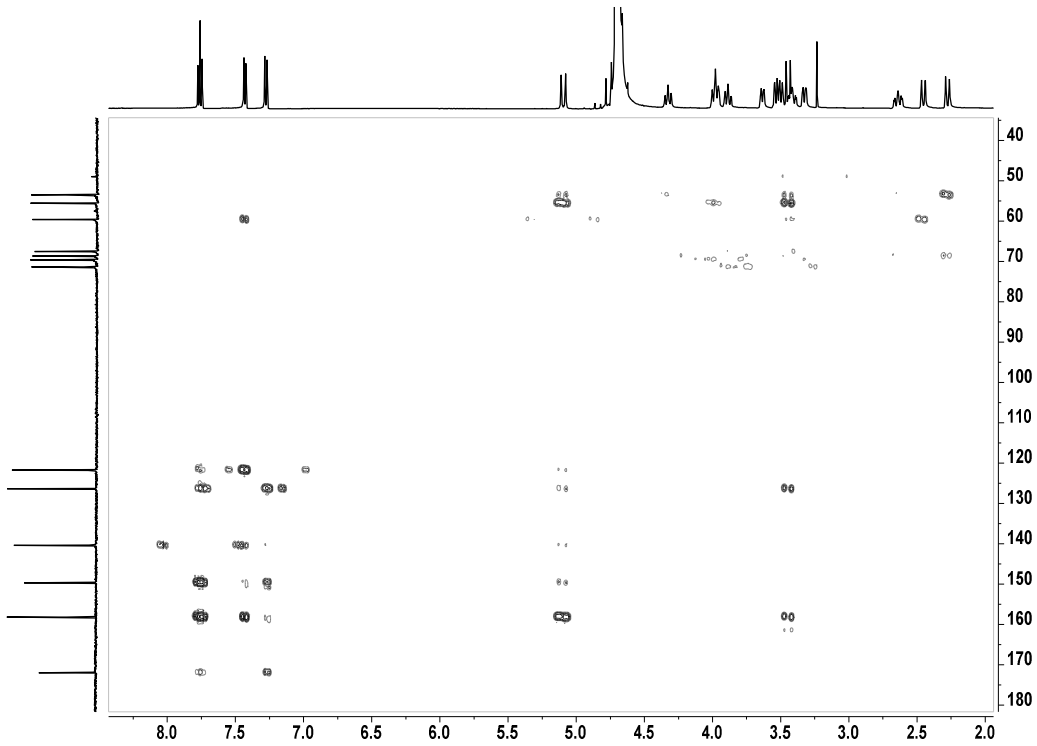
[La(dpa18c6)]: ^{13}C-RMN (D_2O, 75.5 MHz) (δ / ppm)



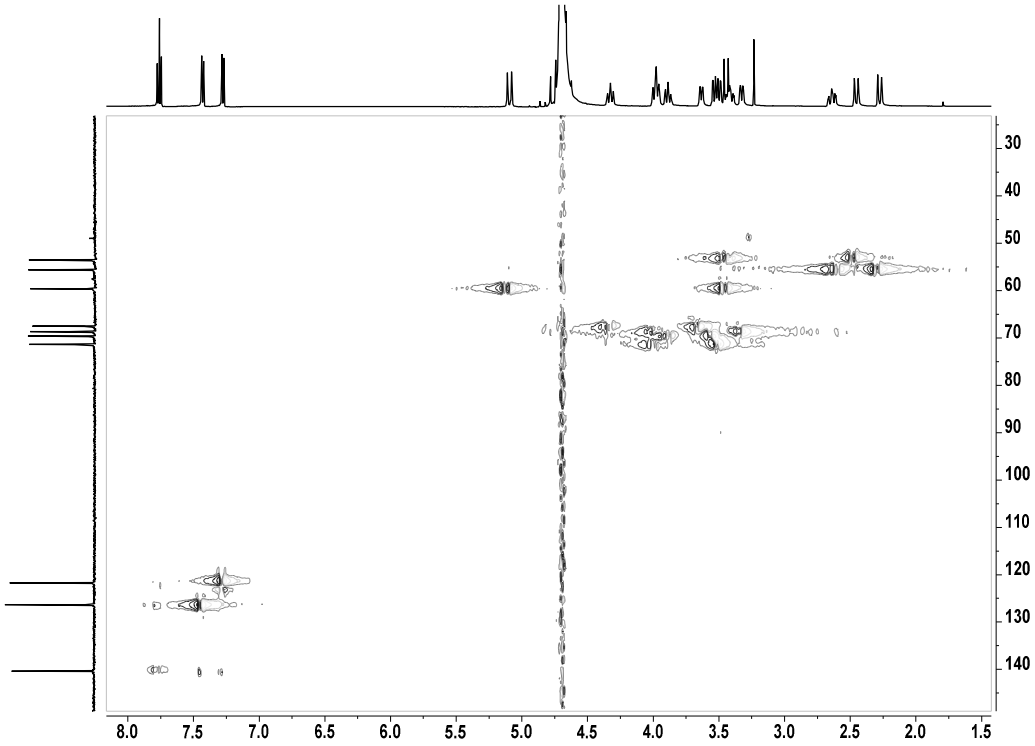
[La(dpa18c6)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



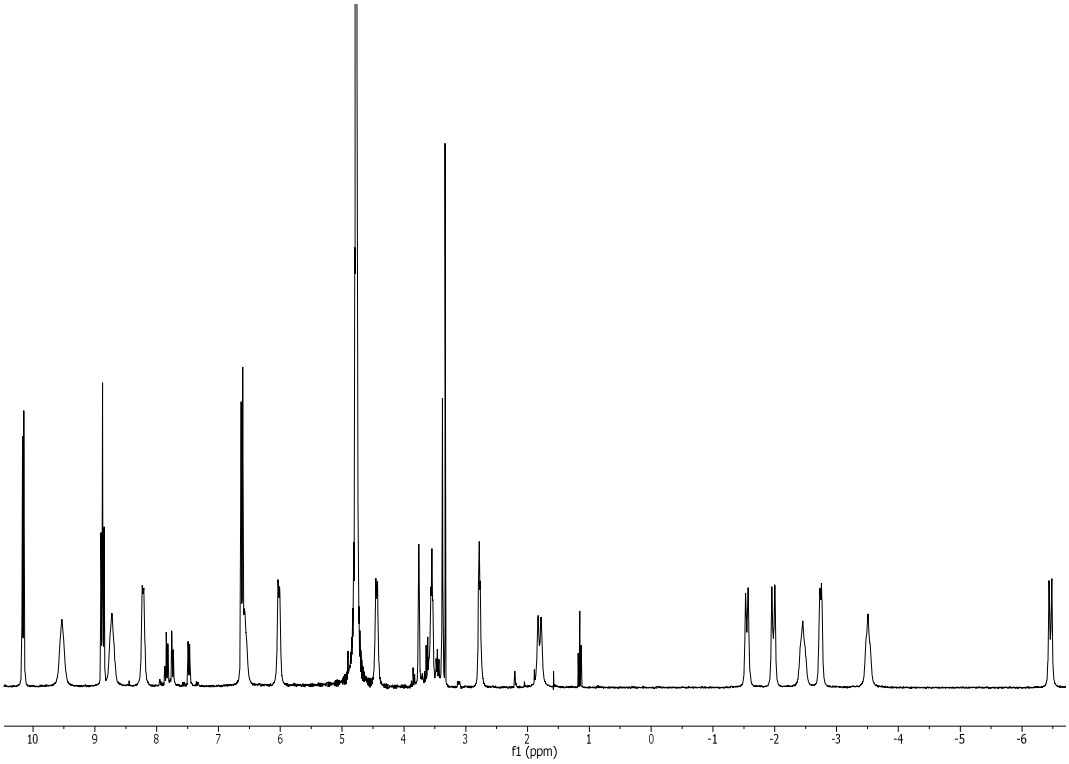
[La(dpa18c6)]: ^{1}H-HMBC (D_2O, 500 MHz) (δ / ppm)



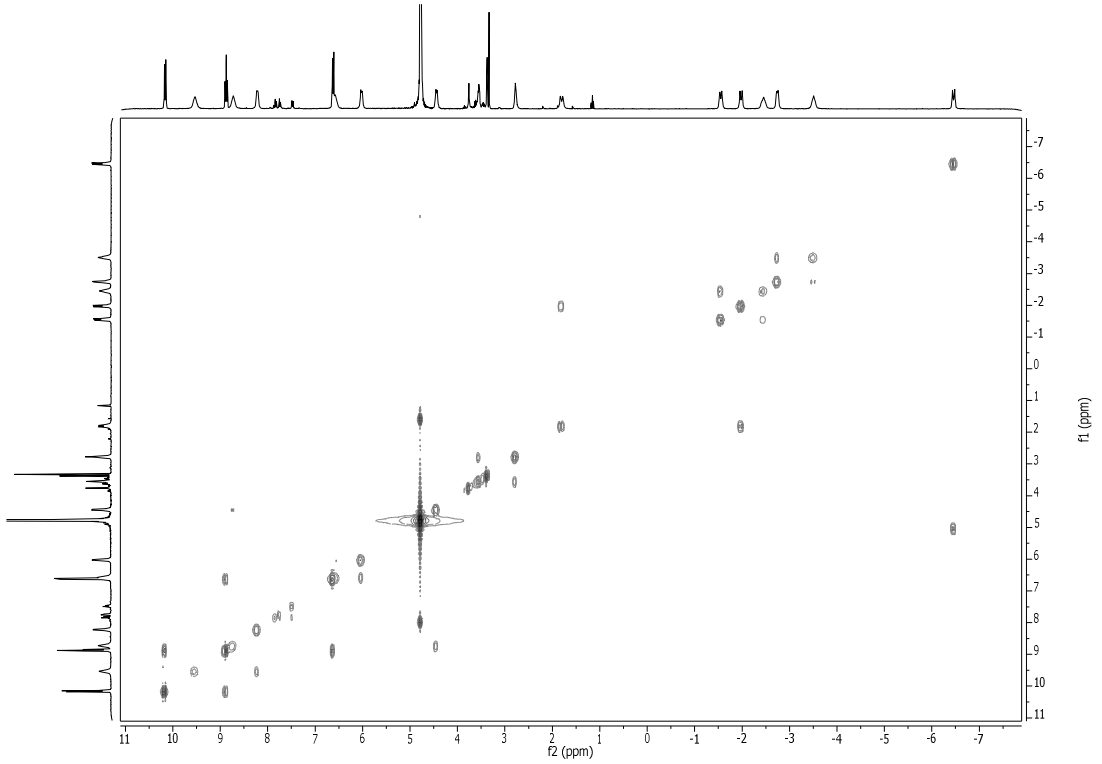
[La(dpa18c6)]: ^{1}H-HSQC (D_2O, 500 MHz) (δ / ppm)



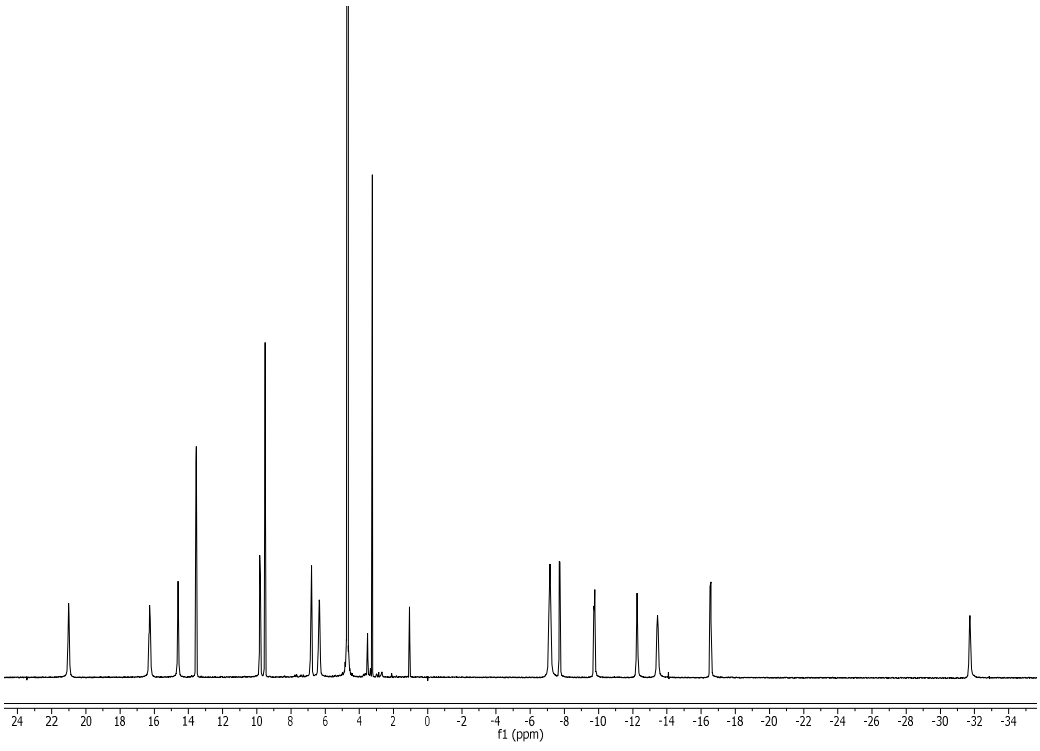
[Ce(dpa18c6)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



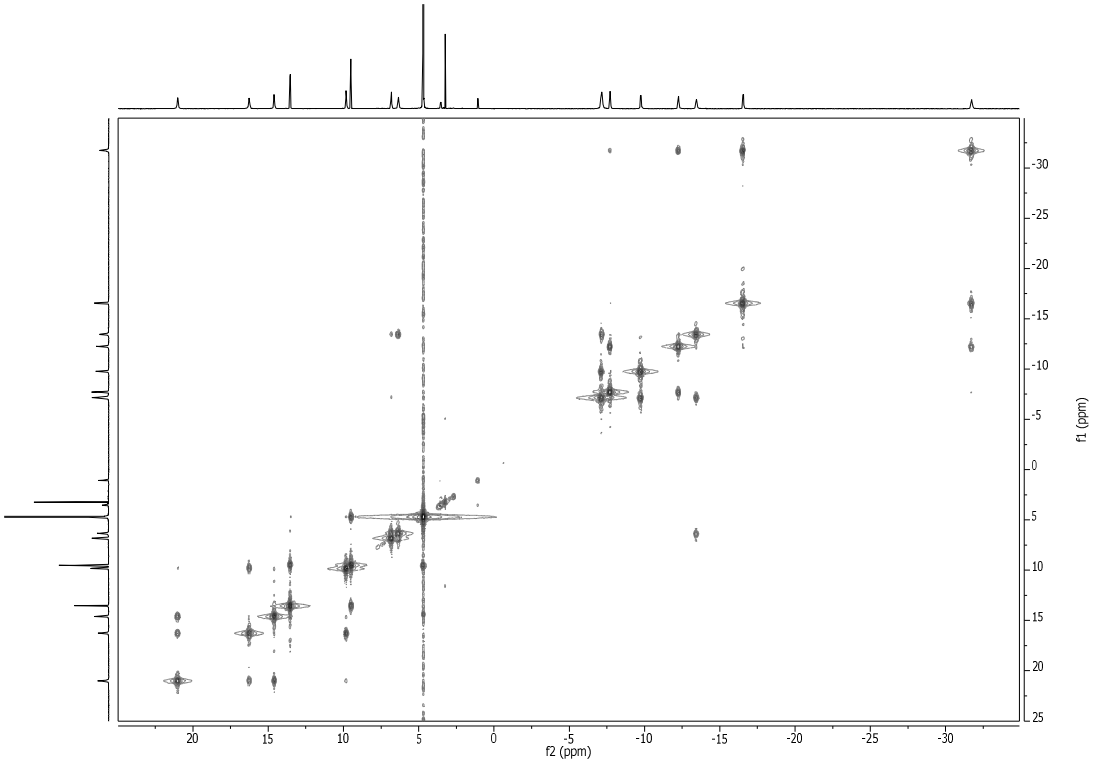
[Ce(dpa18c6)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



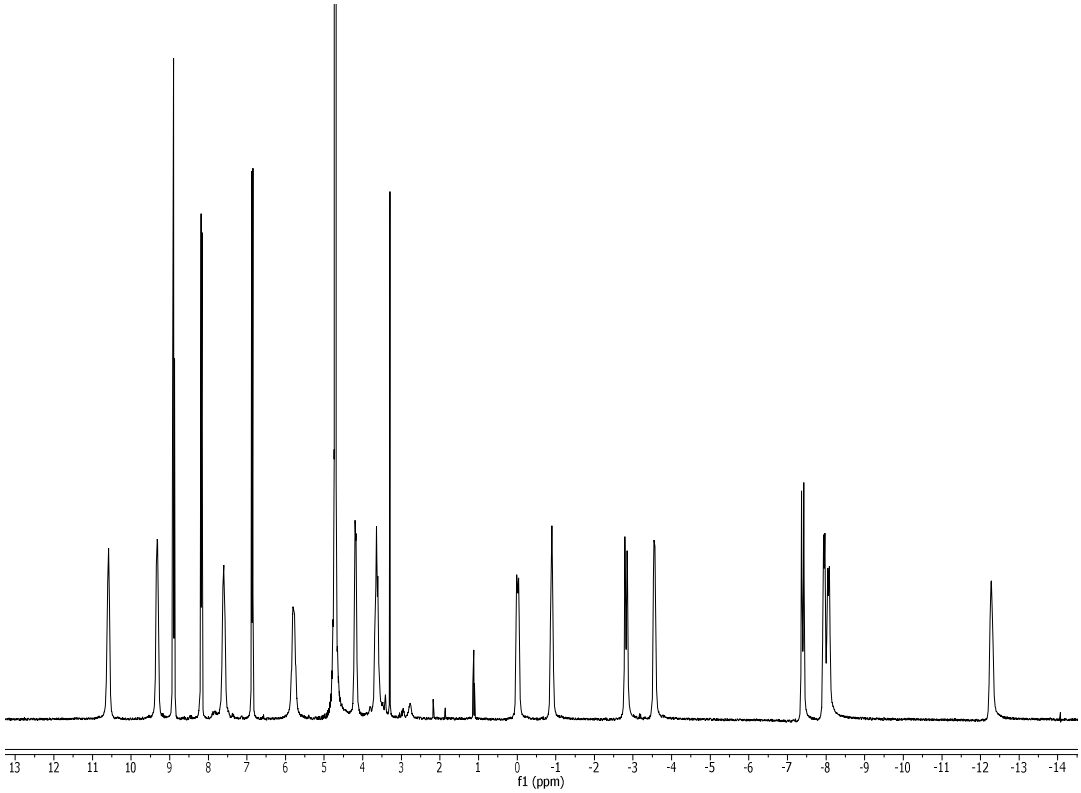
[Pr(dpa18c6)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



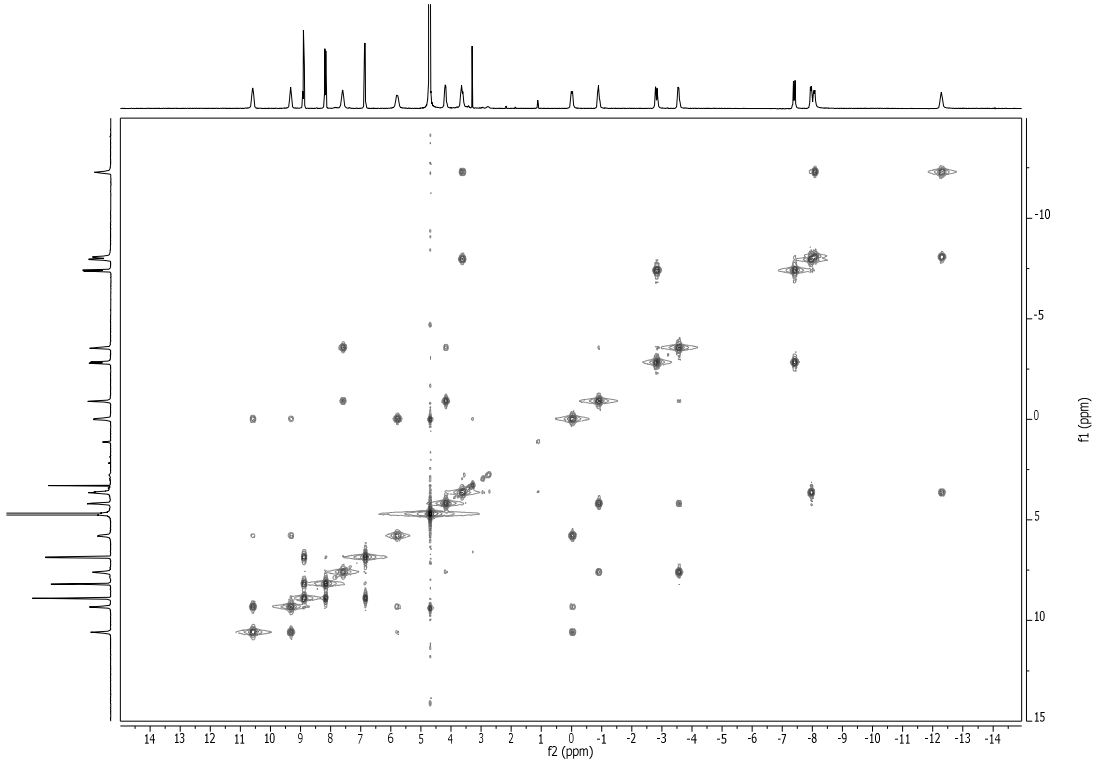
[Pr(dpa18c6)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



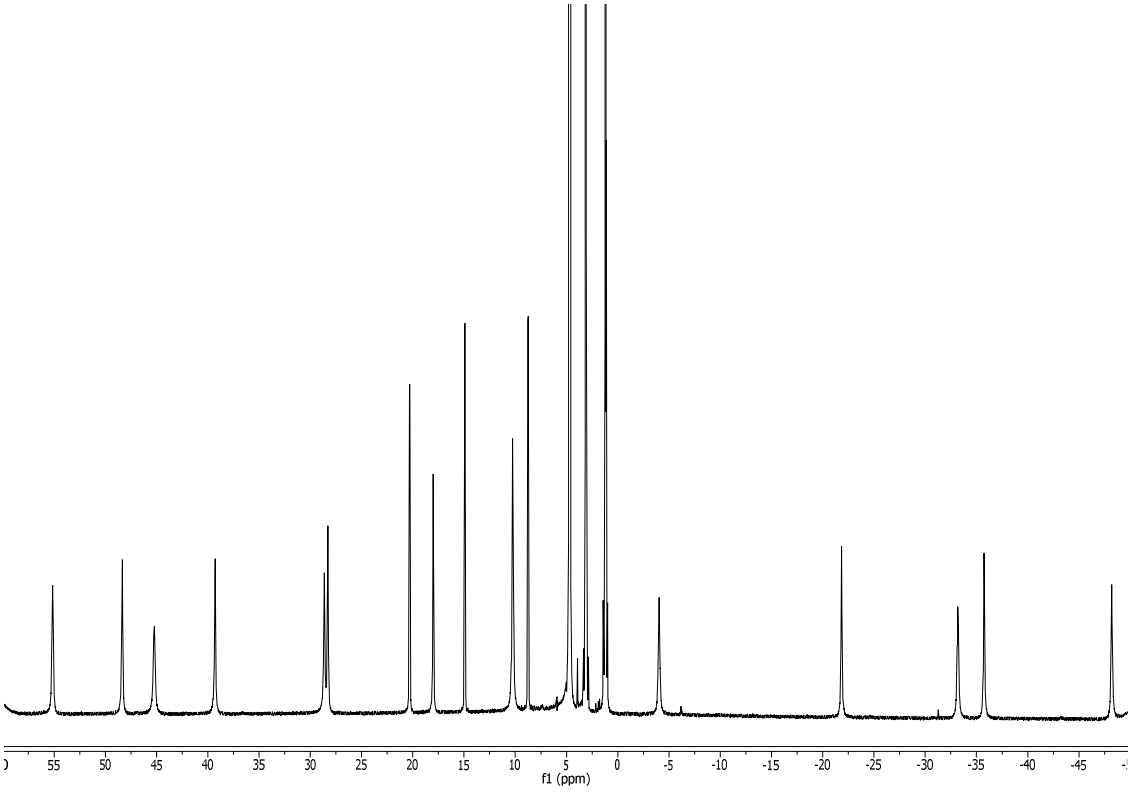
[Eu(dpa18c6)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



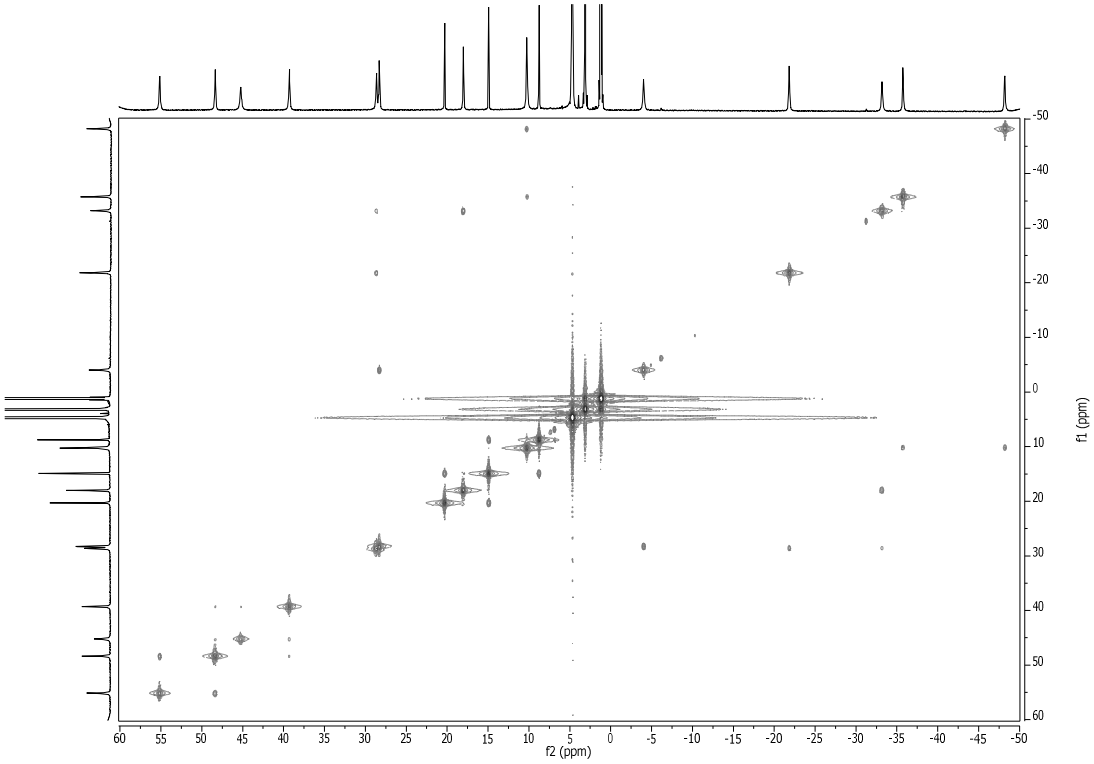
[Eu(dpa18c6)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



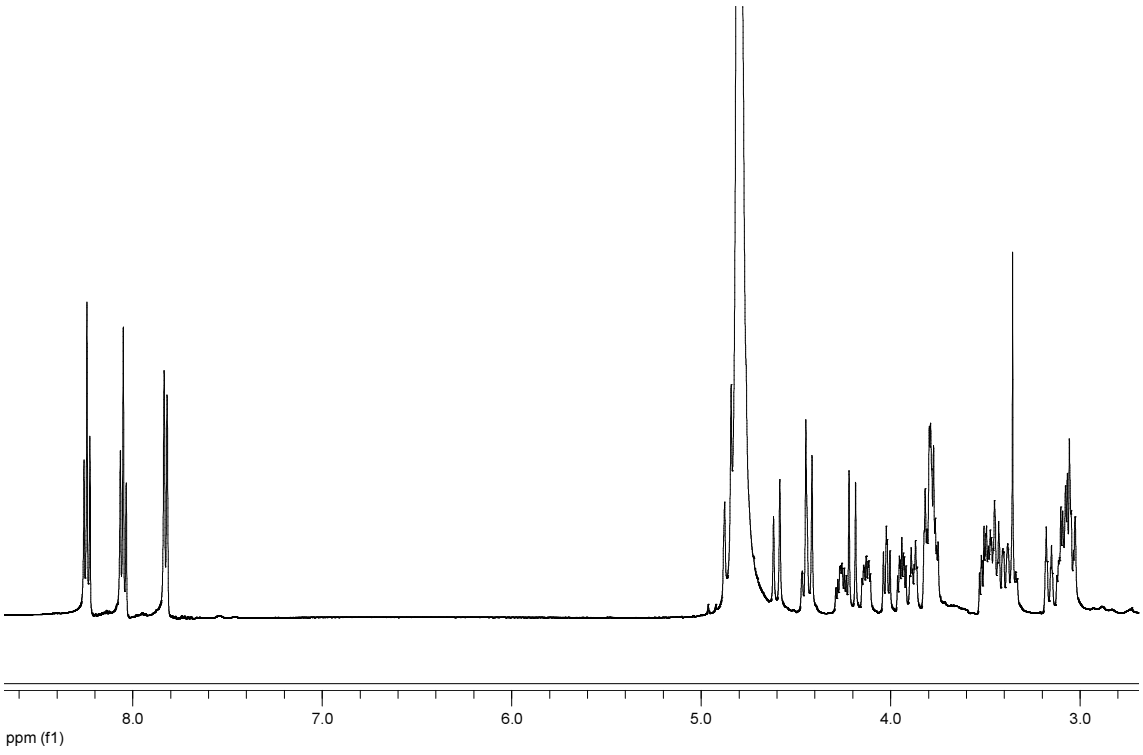
[Yb(dpa18c6)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



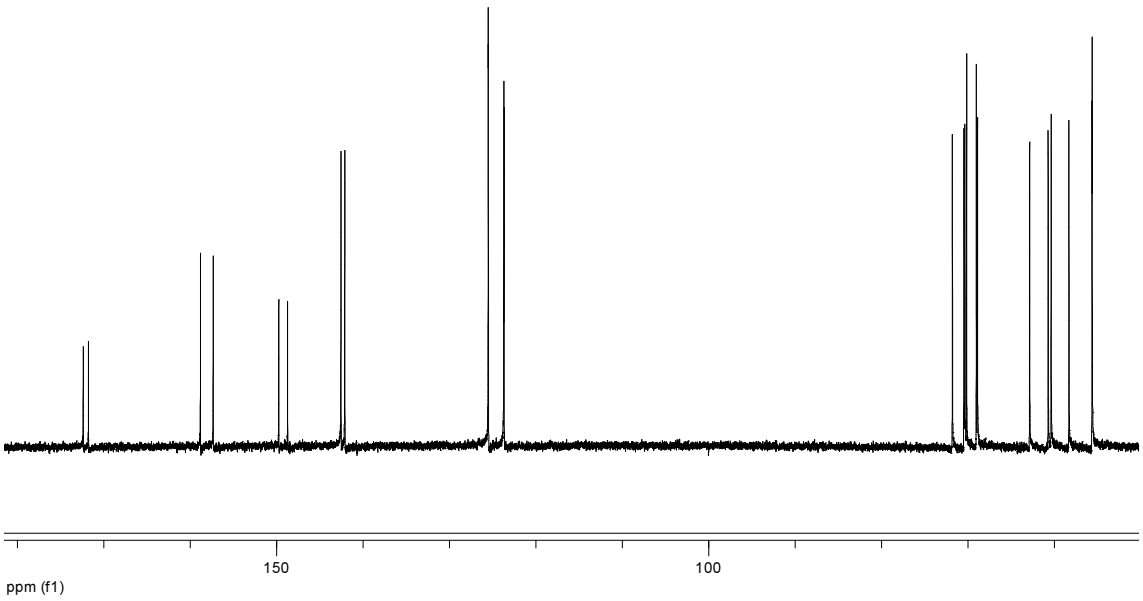
[Yb(dpa18c6)]: ^{1}H-COSY (D_2O, 300 MHz) (δ / ppm)



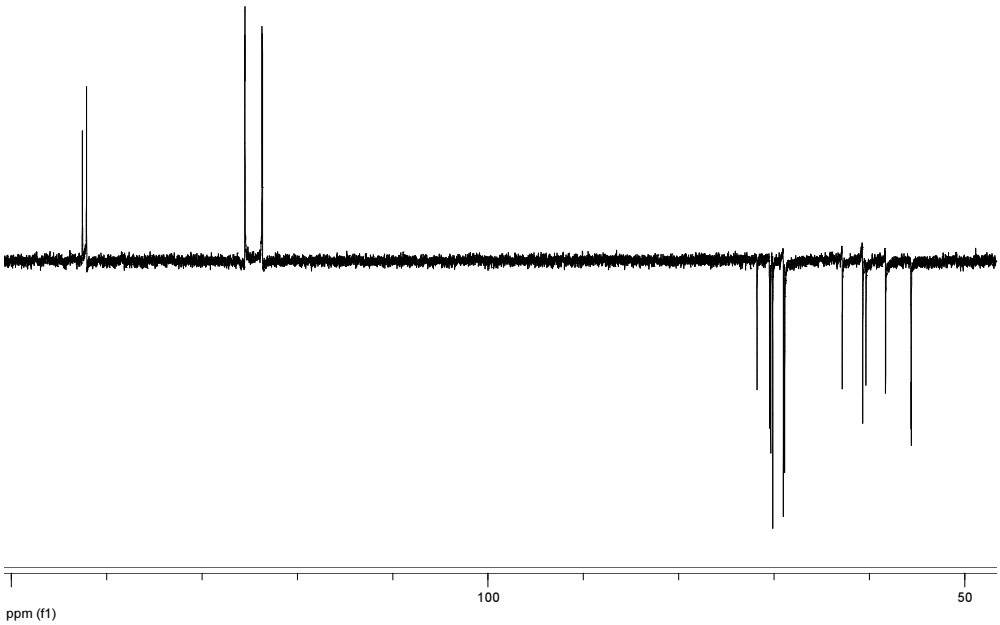
[Lu(dpa15c5)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



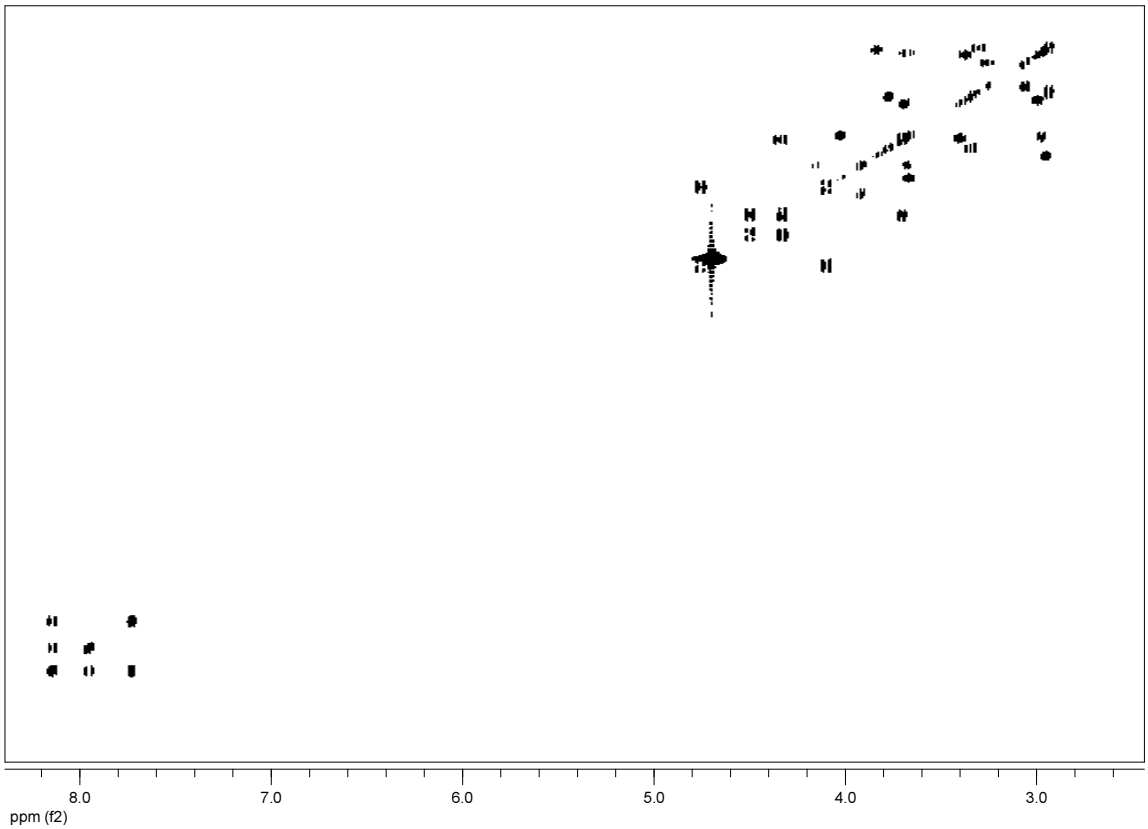
[Lu(dpa15c5)]: ^{13}C-RMN (D_2O, 128.5 MHz) (δ / ppm)



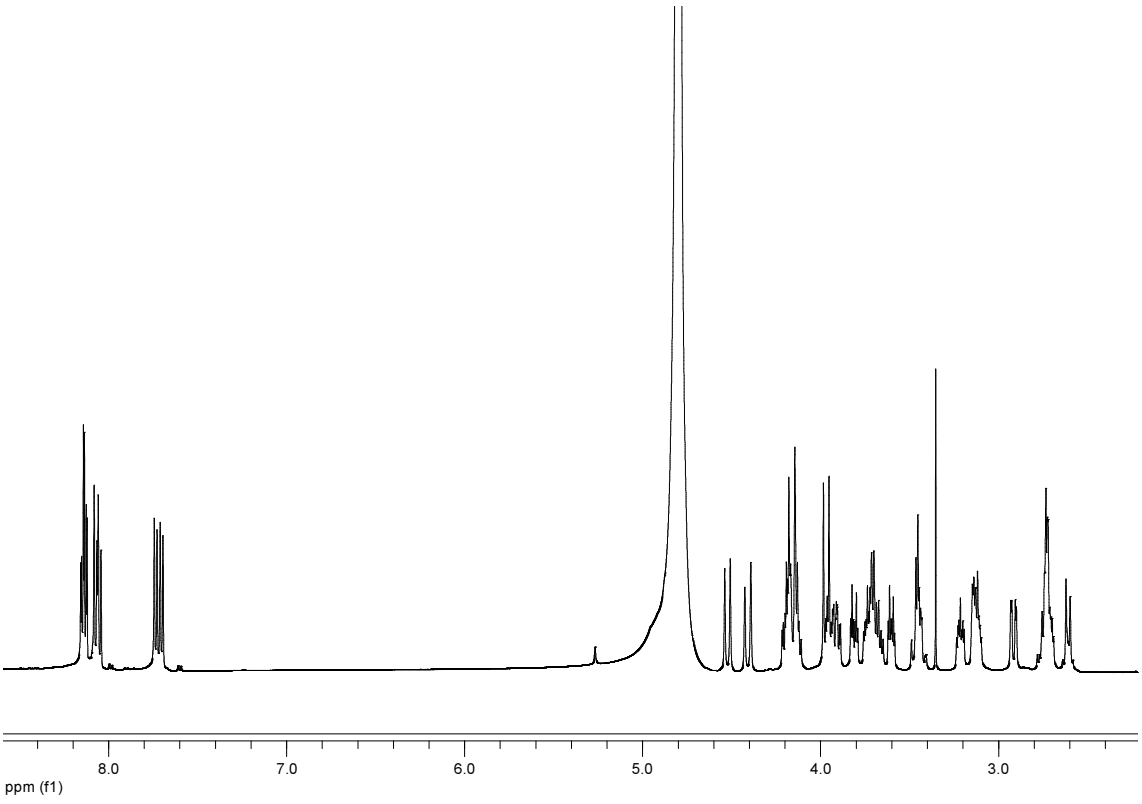
[Lu(dpa15c5)]: ^{13}C- DEPT (D_2O, 128.5 MHz) (δ / ppm)



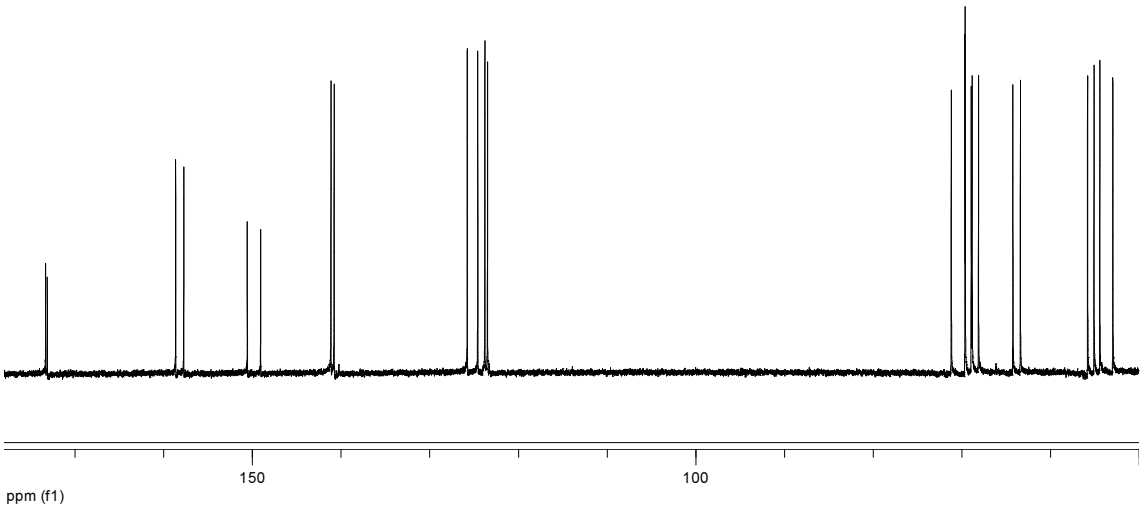
[Lu(dpa15c5)]: ^{1}H-COSY (D_2O, 500 MHz) (δ / ppm)



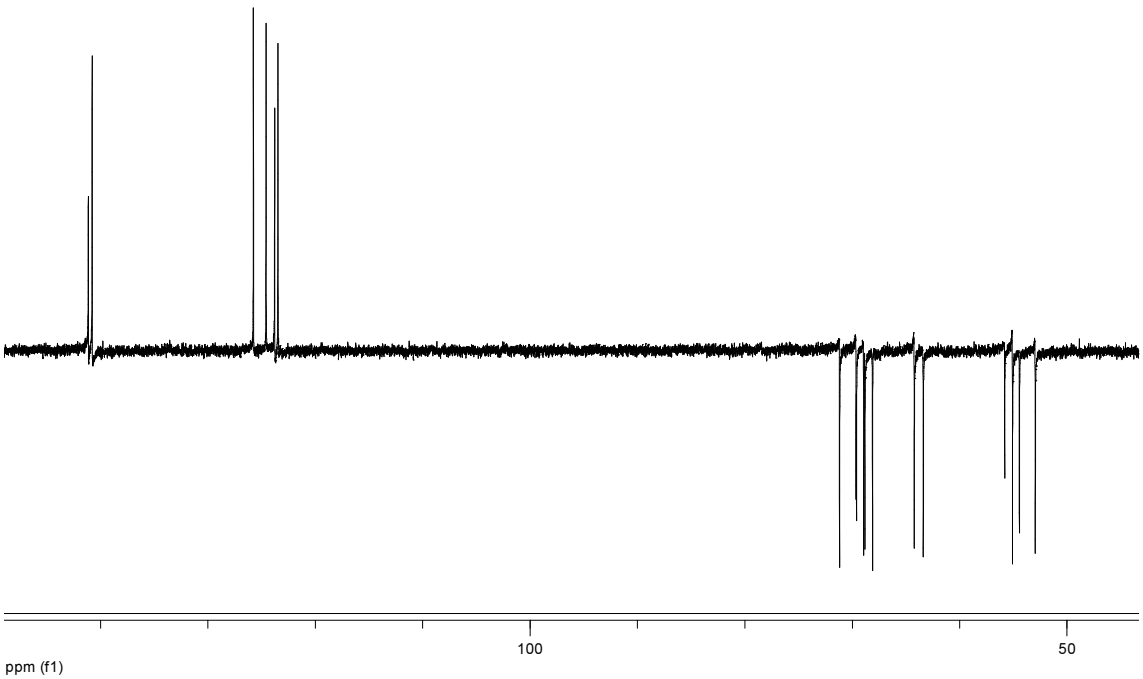
[La(dpa15c5)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



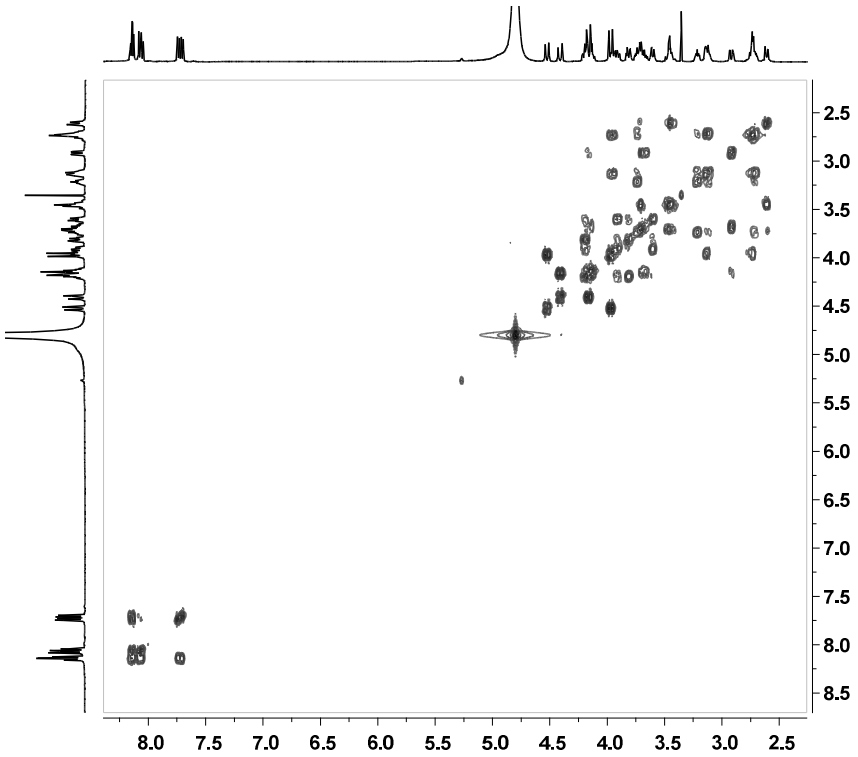
[La(dpa15c5)]: ^{13}C-RMN (D_2O, 128.5 MHz) (δ / ppm)



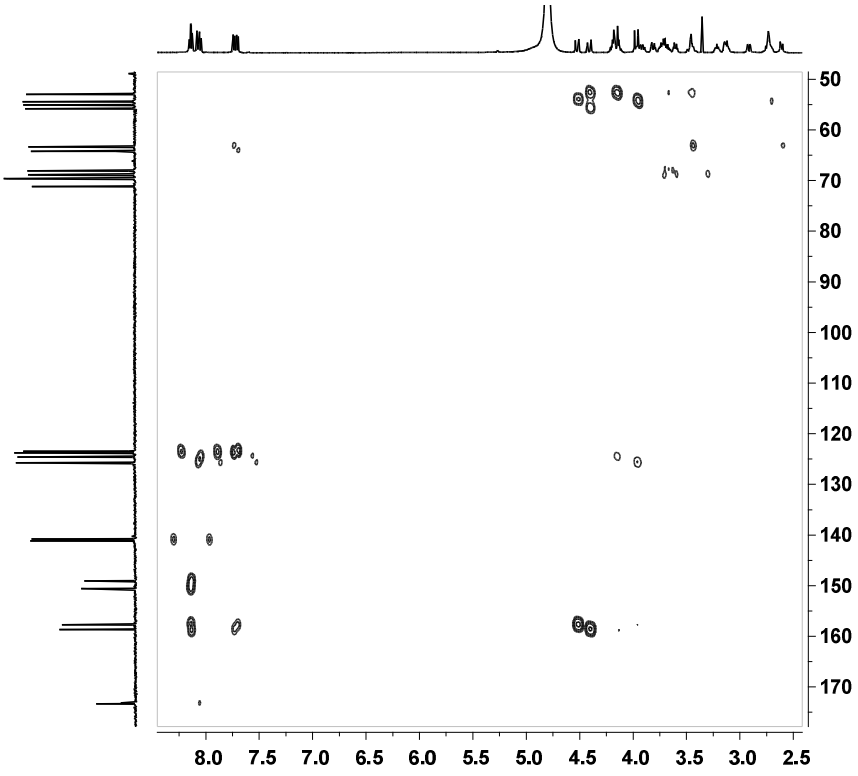
[La(dpa15c5)]: ^{13}C- DEPT (D_2O, 128.5 MHz) (δ / ppm)



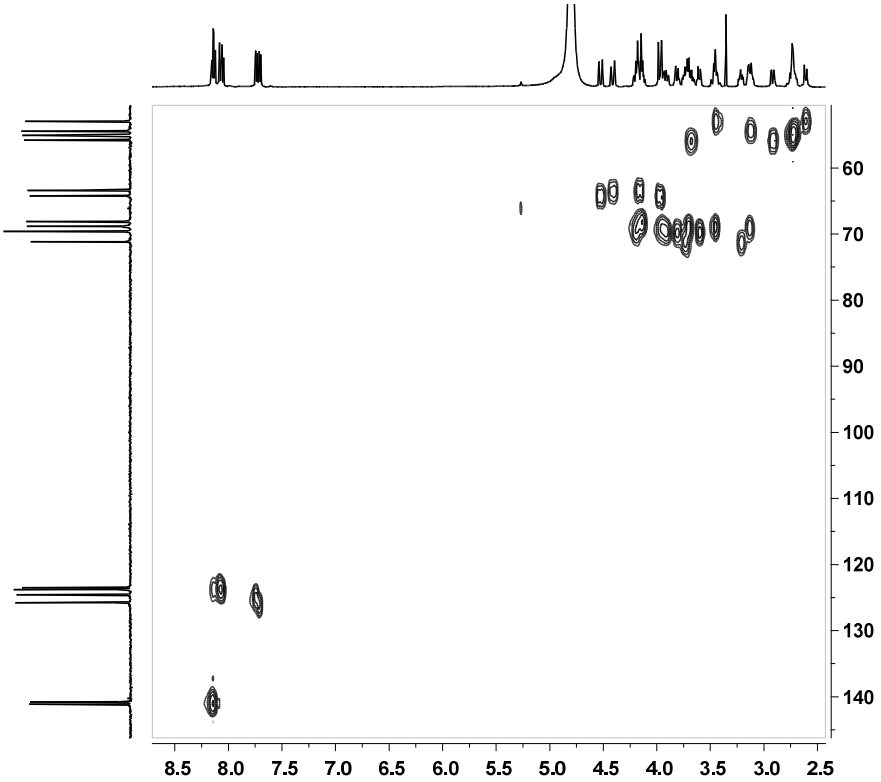
[La(dpa15c5)]: ^{1}H-COSY (D_2O, 500 MHz) (δ / ppm)



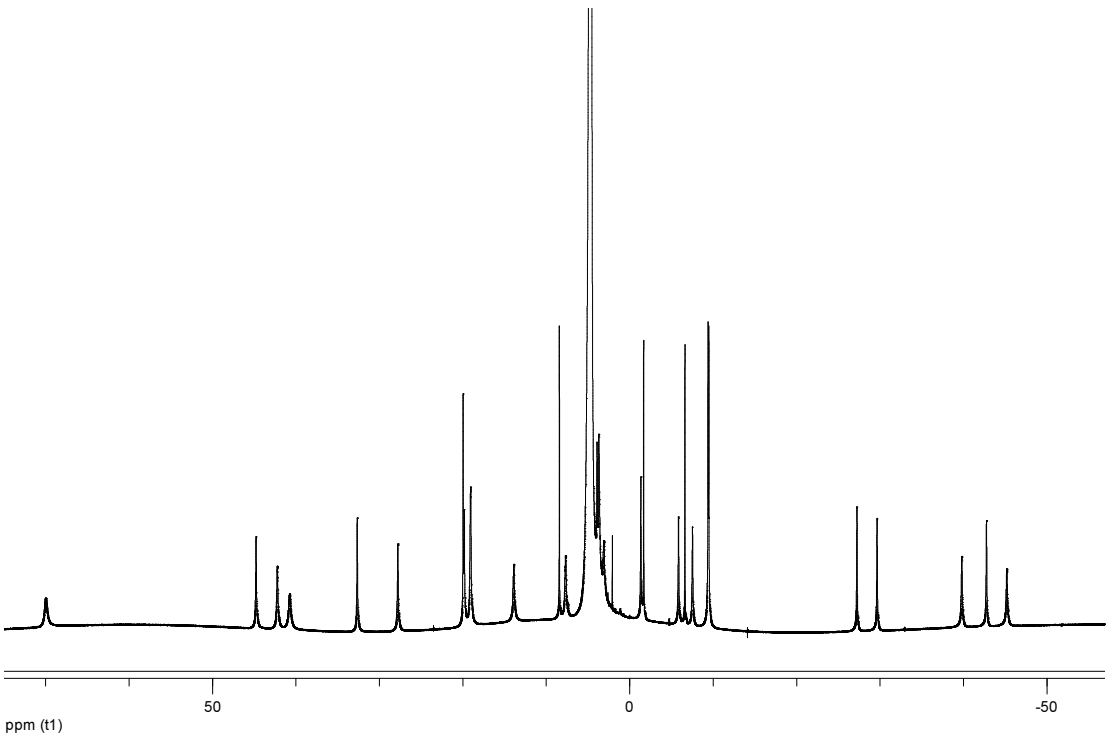
[La(dpa15c5)]: HMBC (D_2O, 300 MHz) (δ / ppm)



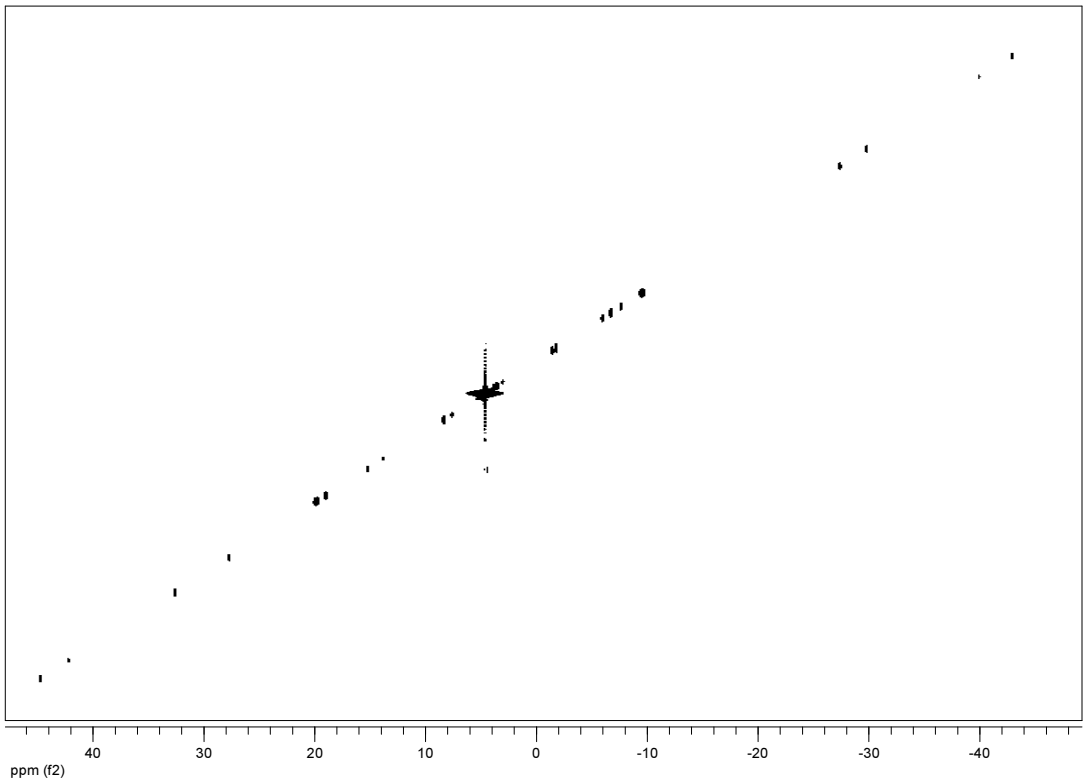
[La(dpa15c5)]: HSQC (D_2O, 300 MHz) (δ / ppm)



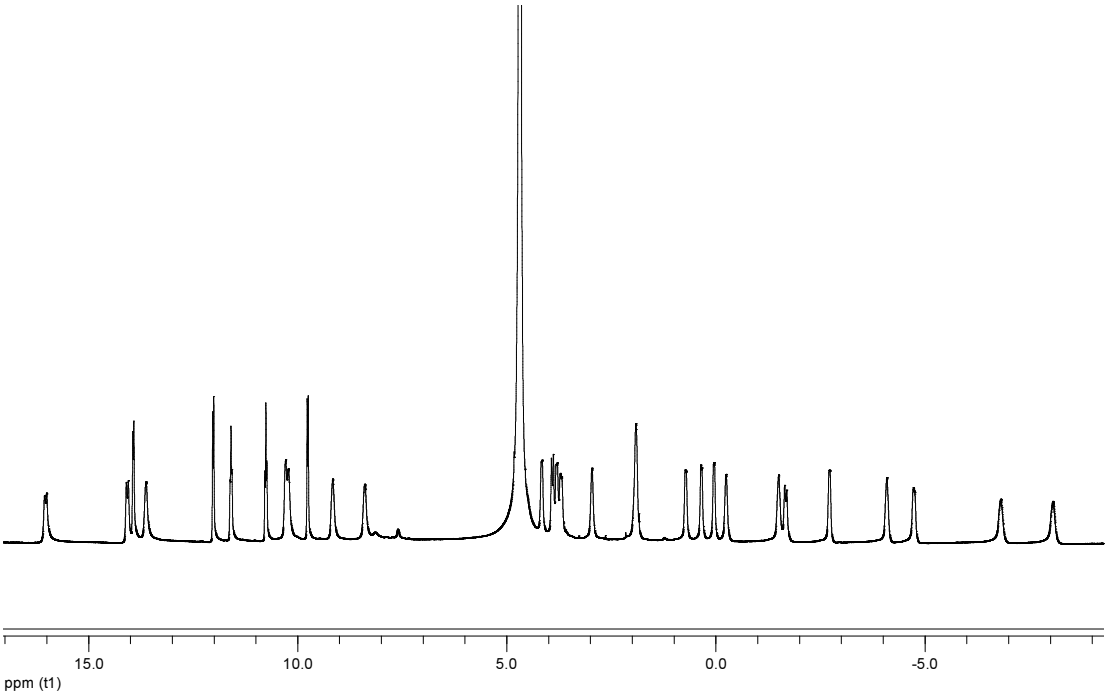
[Yb(dpa15c5)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



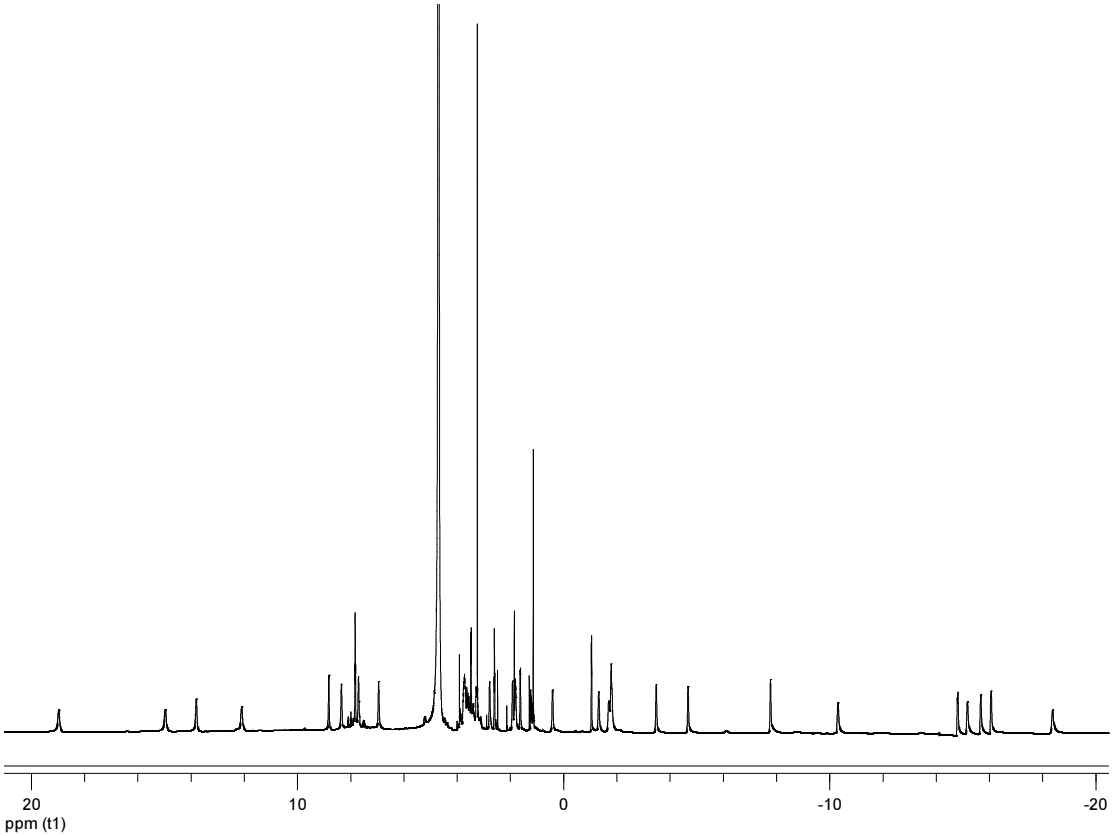
[Yb(dpa15c5)]: ^{1}H-COSY (D_2O, 500 MHz) (δ / ppm)



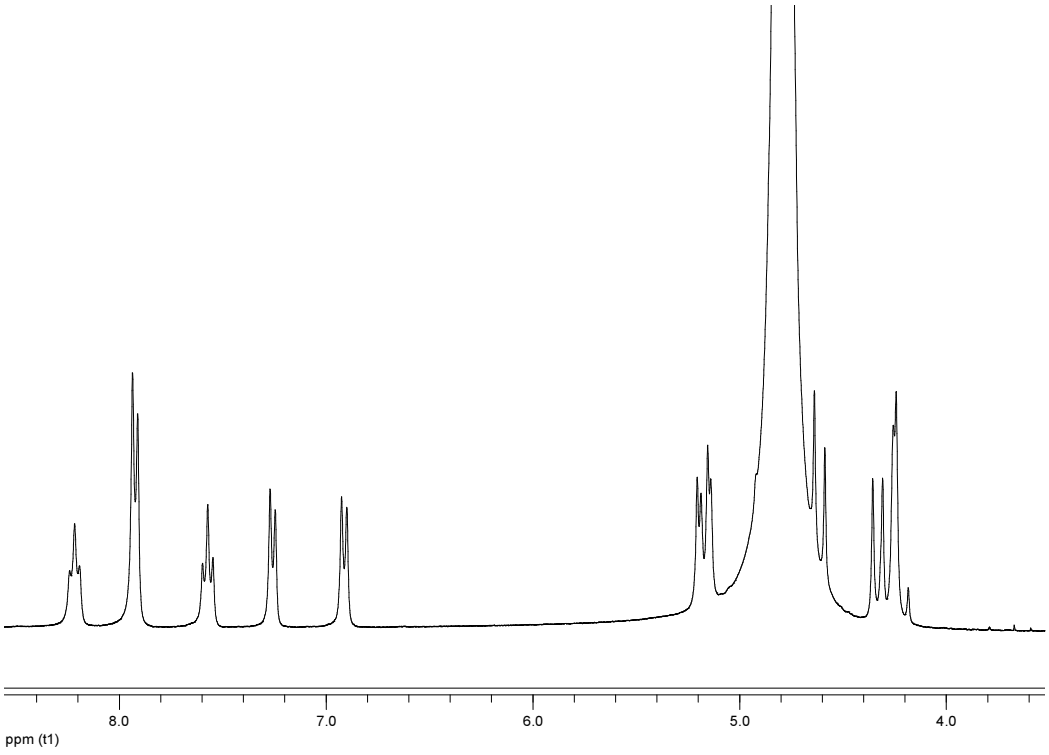
[Ce(dpa15c5)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



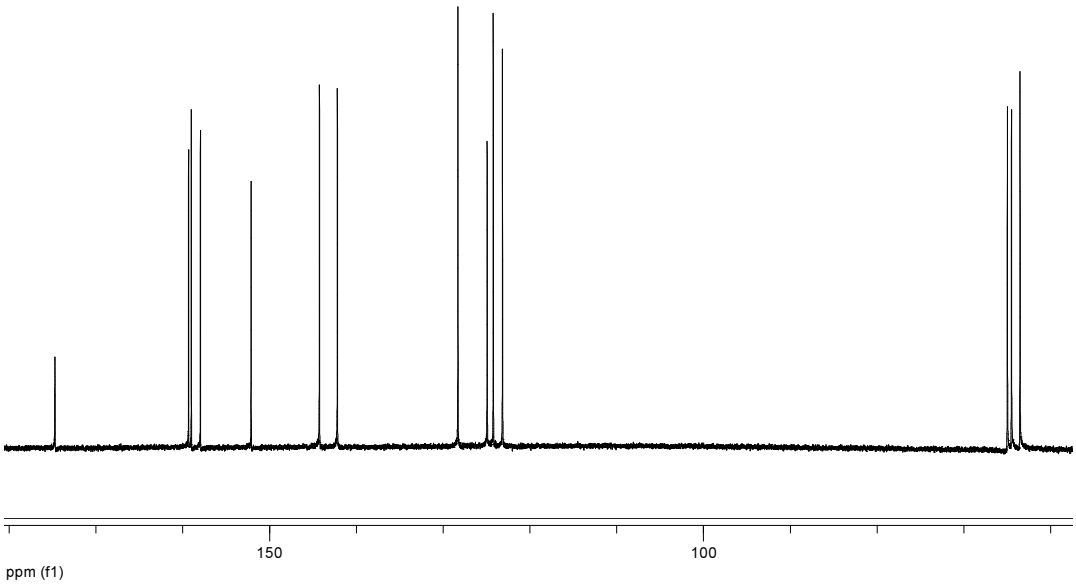
[Eu(dpa15c5)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



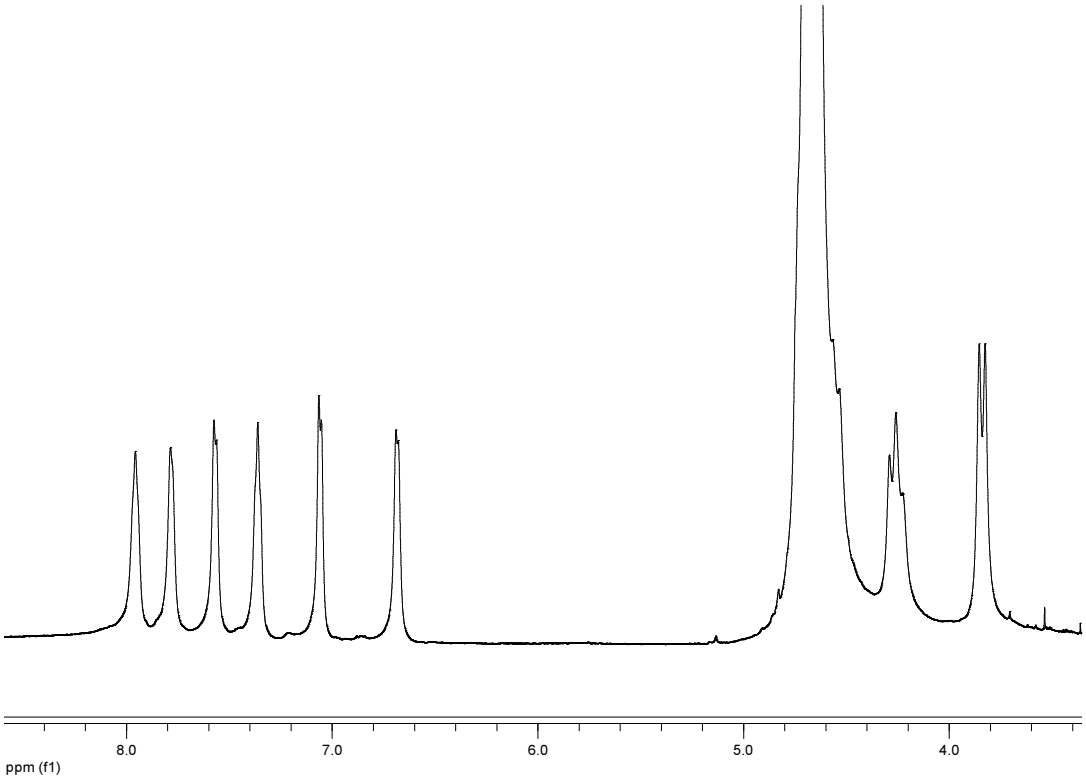
[Lu(dpabp)]: ^{1}H-RMN (D_2O, 300 MHz) (δ / ppm)



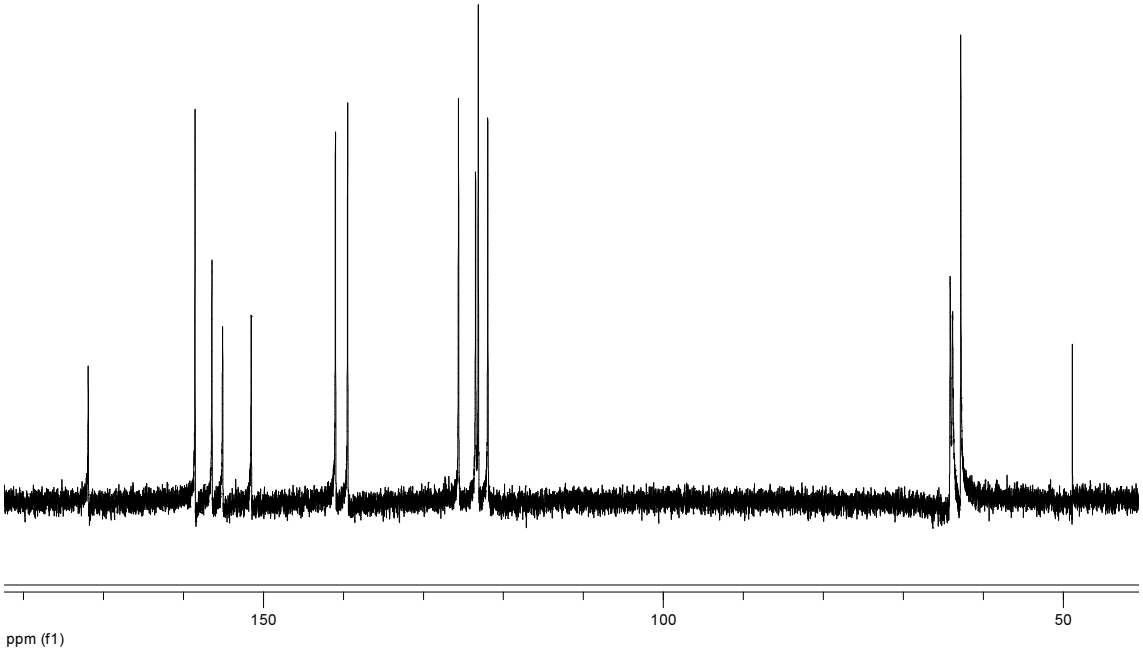
[Lu(dpabp)]: ^{13}C-RMN (D_2O, 128.5 MHz) (δ / ppm)



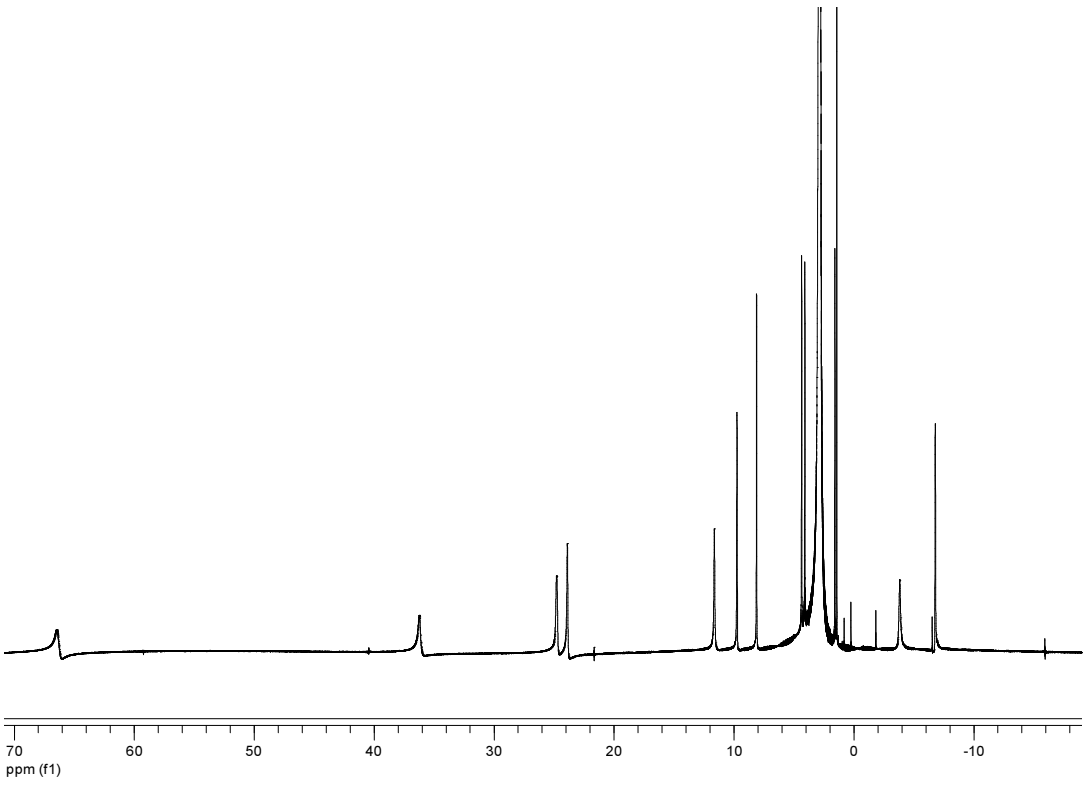
[La(dpabp)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



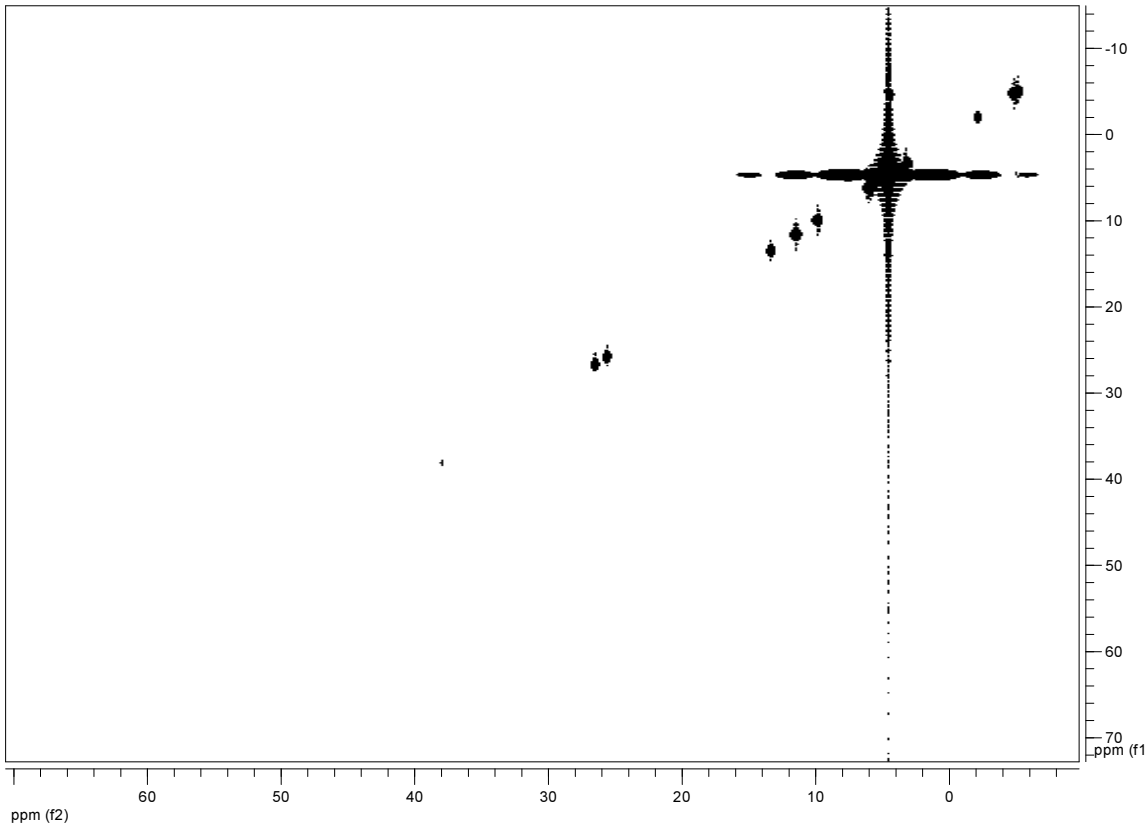
[La(dpabp)]: ^{13}C-RMN (D_2O, 128.5 MHz) (δ / ppm)



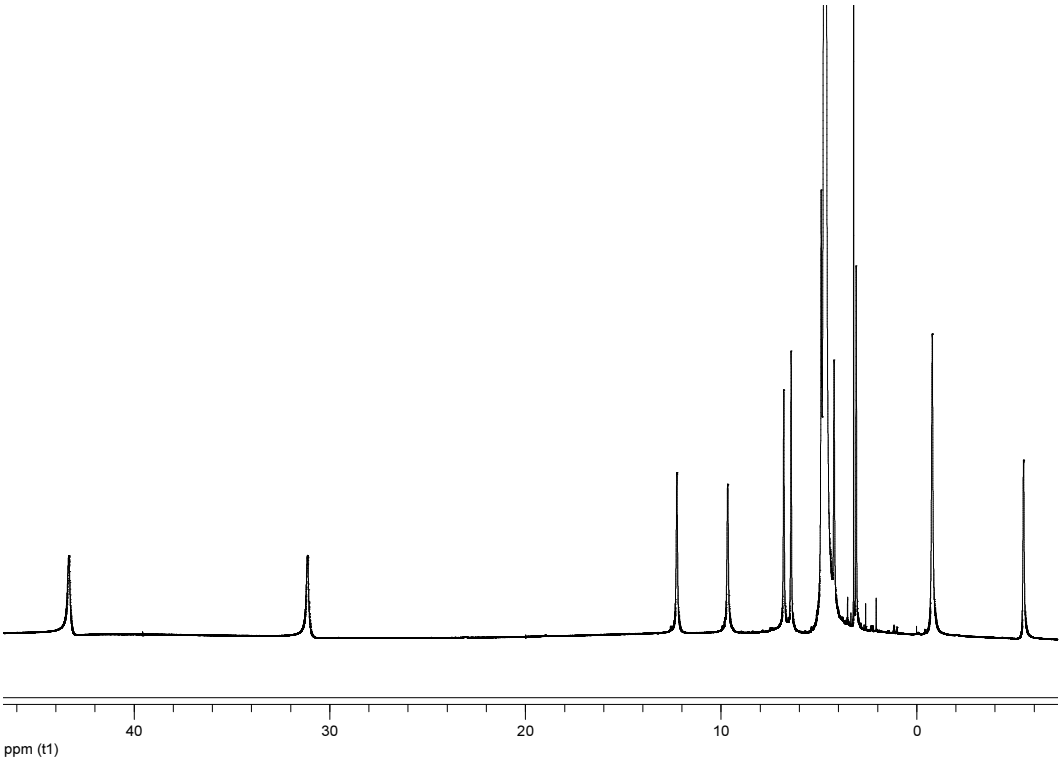
[Yb(dpabp)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



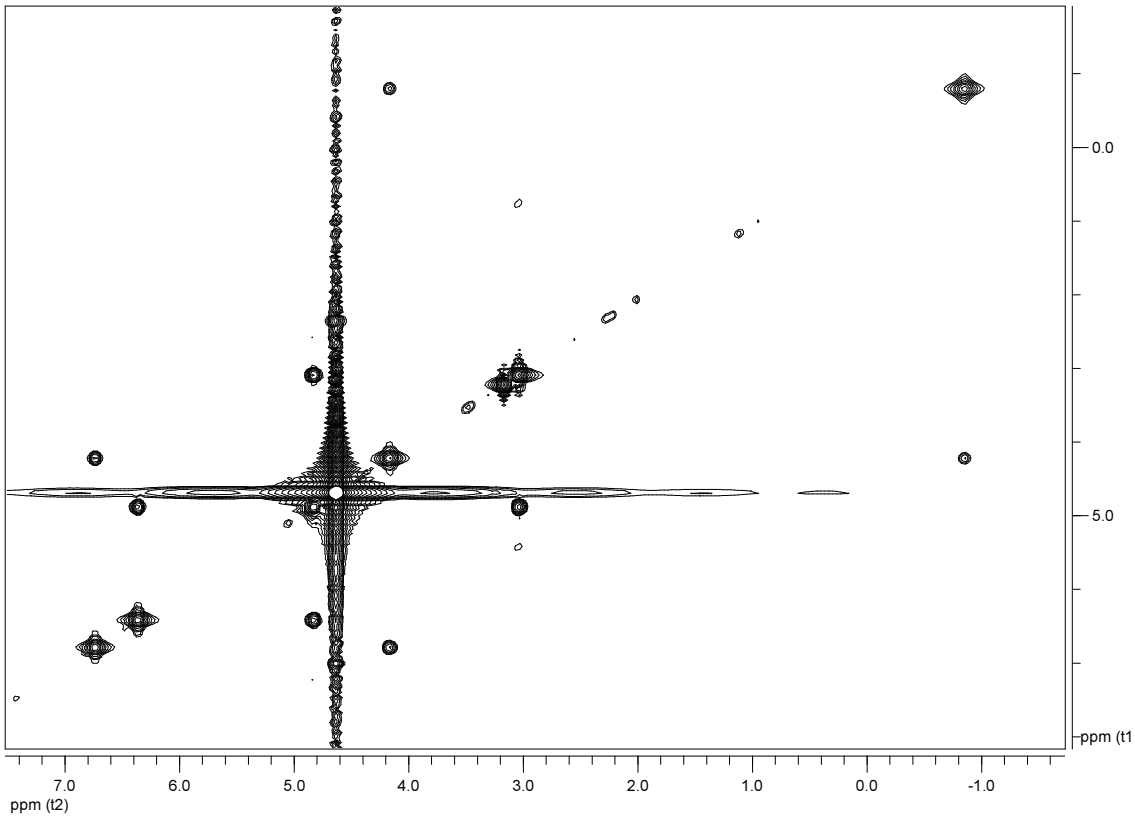
[Yb(dpabp)]: ^{1}H-COSY (D_2O, 500 MHz) (δ / ppm)



[Eu(dpabp)]: ^{1}H-RMN (D_2O, 500 MHz) (δ / ppm)



[Eu(dpabp)]: ^{1}H-COSY (D_2O, 500 MHz) (δ / ppm)



VI.2: TABLAS DE GEOMETRÍAS CALCULADAS

[Gd(dpa12c4)(H_2O)]$^+$ (vacío) **Λ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.000251	-0.108675	-0.001307
2	7	1.829351	1.565156	1.353210
3	6	1.131015	2.463423	2.315638
4	6	-0.307818	2.021394	2.580340
5	6	-1.710657	2.916421	0.758529
6	6	-2.594144	2.354692	-0.351016
7	7	-1.830748	1.563454	-1.354185
8	6	-1.133685	2.462327	-2.317050
9	6	0.306181	2.023002	-2.580893
10	6	1.709241	2.918822	-0.759170
11	6	2.592667	2.356844	0.350383
12	6	2.716917	0.581845	2.037575
13	6	-2.717897	0.579059	-2.037603
14	8	-0.003296	-2.747422	-0.004719
15	1	1.125655	3.475305	1.899149
16	1	1.675280	2.523797	3.268579
17	1	-0.348125	1.052743	3.083905
18	1	-0.834344	2.761698	3.194300
19	1	-1.005122	3.670159	0.383325
20	1	-2.345007	3.396580	1.514556
21	1	-3.332374	1.700162	0.113942
22	1	-3.142177	3.179812	-0.830976
23	1	-1.130412	3.474519	-1.901288
24	1	-1.677671	2.520904	-3.270247
25	1	0.348709	1.054575	-3.084730
26	1	0.831738	2.764461	-3.194272
27	1	1.004300	3.673237	-0.384184
28	1	2.343791	3.398258	-1.515483
29	1	3.330978	1.702465	-0.114692
30	1	3.140589	3.181902	0.830605
31	1	3.548944	1.083364	2.555385
32	1	2.118205	0.071661	2.802809
33	1	-3.550570	1.079610	-2.555297
34	1	-2.119188	0.068902	-2.802868
35	1	0.083949	-3.315642	-0.787061
36	1	-0.075599	-3.316122	0.778712
37	8	-1.013067	1.815355	1.342076
38	8	1.010798	1.818018	-1.342084
39	6	3.260882	-0.431848	1.041001
40	6	4.548753	-0.964524	1.090430
41	6	4.947966	-1.842725	0.076414
42	1	5.228340	-0.693990	1.892565
43	6	2.807625	-1.557991	-0.958361
44	6	4.076324	-2.136898	-0.972381
45	1	5.944614	-2.273942	0.096835
46	1	4.348870	-2.787313	-1.795602
47	6	-3.260572	-0.434305	-1.039920
48	6	-4.548127	-0.967818	-1.088116
49	6	-2.805544	-1.557826	0.960513
50	6	-4.946374	-1.844852	-0.072702
51	1	-5.228254	-0.698702	-1.890272
52	6	-4.074152	-2.136908	0.976185
53	1	-5.942799	-2.276634	-0.092044
54	1	-4.346113	-2.785803	1.800792
55	7	-2.419415	-0.757759	-0.045878

56	7	2.420516	-0.756764	0.046765
57	6	1.784048	-1.783089	-2.078374
58	8	0.711499	-1.041422	-1.985334
59	8	2.029866	-2.621459	-2.932565
60	6	-1.782058	-1.780504	2.081121
61	8	-2.031775	-2.610901	2.941796
62	8	-0.705743	-1.044746	1.982401

E(RB3LYP) = -1636.7344721 Hartree
Corrección de punto cero = 0.502559 Hartrees
Suma de las entalpías electrónicas y térmicas = -1636.199202 Hartrees
Suma de las energías libres y térmicas = -1636.293401 Hartrees

[Gd(dpa12c4)(H_2O)]$^+$ (vacío) Δ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.000126	-0.210050	-0.036982
2	7	1.403111	1.555547	-1.548430
3	6	1.983146	2.663070	-0.737134
4	6	2.279801	2.308046	0.723613
5	6	0.826248	1.929009	2.649166
6	6	-0.390372	1.089941	3.065898
7	7	-1.399970	0.946746	1.979890
8	6	-1.981278	2.261665	1.585582
9	6	-2.278626	2.416412	0.090274
10	6	-0.824693	2.702622	-1.851254
11	6	0.392770	2.052366	-2.524181
12	6	2.451230	0.765190	-2.249859
13	6	-2.446472	-0.033180	2.377850
14	8	0.000560	-2.715517	-0.471625
15	1	1.267256	3.486338	-0.733422
16	1	2.903871	3.042801	-1.203948
17	1	3.149318	1.652941	0.834048
18	1	2.480826	3.238023	1.270020
19	1	0.649710	3.007142	2.762140
20	1	1.674051	1.657661	3.290319
21	1	-0.050428	0.081260	3.308511
22	1	-0.826667	1.539917	3.971653
23	1	-1.266040	3.039794	1.856815
24	1	-2.902067	2.463622	2.152659
25	1	-3.148874	1.837820	-0.233524
26	1	-2.478201	3.476070	-0.112586
27	1	-0.648873	3.756428	-1.596495
28	1	-1.671720	2.661431	-2.547197
29	1	0.053933	1.182561	-3.090281
30	1	0.827444	2.779865	-3.227811
31	1	1.944770	0.141495	-2.996710
32	1	3.146198	1.421349	-2.795049
33	1	-1.938464	-0.871838	2.869659
34	1	-3.139204	0.401212	3.114129
35	1	-0.211518	-3.138743	-1.318507
36	1	0.211971	-3.399142	0.183538
37	8	1.127787	1.659204	1.275356
38	8	-1.127626	1.988538	-0.647324
39	6	3.211670	-0.138472	-1.294753
40	6	4.570283	-0.431790	-1.412379
41	6	5.150931	-1.296043	-0.477986
42	1	5.161748	0.004850	-2.211263

43	6	3.027627	-1.466350	0.618385
44	6	4.375999	-1.817984	0.557967
45	1	6.205798	-1.544014	-0.552062
46	1	4.780953	-2.474070	1.319989
47	6	-3.209740	-0.563945	1.176596
48	6	-4.567963	-0.881272	1.191689
49	6	-3.030057	-1.171446	-1.071995
50	6	-5.150699	-1.381587	0.022369
51	1	-5.157630	-0.739807	2.092191
52	6	-4.378318	-1.523712	-1.130554
53	1	-6.205300	-1.641249	0.011177
54	1	-4.784954	-1.885636	-2.067997
55	7	-2.472431	-0.729154	0.067573
56	7	2.472164	-0.666623	-0.307490
57	6	2.110151	-1.936851	1.753032
58	8	0.914612	-1.409921	1.726194
59	8	2.548983	-2.736160	2.565362
60	6	-2.115191	-1.232697	-2.300688
61	8	-2.557259	-1.709053	-3.334645
62	8	-0.918909	-0.746895	-2.100041

E(RB3LYP) = -1636.7437182 Hartrees
Corrección de punto cero = 0.503200 Hartrees
Suma de las entalpías electrónicas y térmicas = -1636.207724 Hartrees
Suma de las energías libres y térmicas = -1636.302012 Hartrees

$[Gd(dpa12c4)(H_2O)]^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	-0.000006	-0.112719	-0.000034
2	7	1.617993	1.224541	1.644616
3	6	0.728511	1.764071	2.704995
4	6	-0.381529	2.669688	2.174500
5	6	-1.756200	2.972724	0.232663
6	6	-2.435728	2.242911	-0.929372
7	7	-1.618070	1.224623	-1.644566
8	6	-0.728580	1.764125	-2.704952
9	6	0.381505	2.669698	-2.174455
10	6	1.756205	2.972661	-0.232602
11	6	2.435698	2.242798	0.929429
12	6	2.526993	0.186984	2.221585
13	6	-2.527133	0.187095	-2.221482
14	8	-0.000428	-2.697705	-0.000414
15	1	1.298933	2.331296	3.458261
16	1	0.271680	0.901327	3.196063
17	1	-1.085167	3.768197	-0.111340
18	1	-2.540130	3.449094	0.836875
19	1	-3.304661	1.723132	-0.522843
20	1	-2.816356	3.000770	-1.632218
21	1	-1.298983	2.331385	-3.458205
22	1	-0.271783	0.901374	-3.196039
23	1	1.085213	3.768166	0.111410
24	1	2.540162	3.448997	-0.836807
25	1	3.304604	1.722981	0.522889
26	1	2.816368	3.000634	1.632277
27	1	3.285377	0.638953	2.877815
28	1	1.910819	-0.477989	2.837926
29	1	-3.285558	0.639087	-2.877651

30	1	-1.911026	-0.477882	-2.837889
31	1	0.120551	-3.263206	-0.779207
32	1	-0.120466	-3.263730	0.778142
33	8	-1.015122	2.053209	1.039850
34	8	1.015079	2.053196	-1.039804
35	6	3.185936	-0.613916	1.109909
36	6	4.483357	-1.123208	1.155449
37	6	4.958923	-1.833597	0.046781
38	1	5.109528	-0.966469	2.028341
39	6	2.862406	-1.456493	-1.047281
40	6	4.147232	-1.998625	-1.076341
41	1	5.965540	-2.241400	0.058481
42	1	4.476898	-2.524308	-1.965221
43	6	-3.186005	-0.613826	-1.109771
44	6	-4.483389	-1.123213	-1.155285
45	6	-2.862284	-1.456575	1.047322
46	6	-4.958837	-1.833733	-0.046649
47	1	-5.109611	-0.966474	-2.028140
48	6	-4.147061	-1.998817	1.076403
49	1	-5.965422	-2.241618	-0.058330
50	1	-4.476625	-2.524633	1.965243
51	7	-2.411331	-0.800364	-0.031593
52	7	2.411319	-0.800455	0.031686
53	6	1.884579	-1.567035	-2.222587
54	8	0.740989	-0.964527	-2.023319
55	8	2.227032	-2.195054	-3.212322
56	6	-1.884347	-1.567225	2.222527
57	8	-2.226809	-2.195076	3.212362
58	8	-0.740791	-0.964651	2.023216
59	1	1.122088	2.829411	-2.967945
60	1	-0.004915	3.652509	-1.877949
61	1	0.004932	3.652484	1.877995
62	1	-1.122107	2.829434	2.967988

E(RB3LYP) = -1636.7443805 Hartrees
Corrección de punto cero = 0.503484 Hartrees
Suma de las entalpías electrónicas y térmicas = -1636.208231 Hartrees
Suma de las energías libres y térmicas = -1636.301426 Hartrees

$[Ho(dpa12c4)(H_2O)]^+$ (vacío) **Λ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	0.000138	-0.070162	-0.000988
2	7	-1.813439	1.540923	-1.364116
3	6	-1.123289	2.442479	-2.329338
4	6	0.326441	2.025346	-2.572851
5	6	1.721428	2.909048	-0.736544
6	6	2.594099	2.333035	0.374002
7	7	1.812509	1.542352	1.363181
8	6	1.121353	2.443613	2.327875
9	6	-0.327504	2.024154	2.572339
10	6	-1.722063	2.907229	0.735778
11	6	-2.594921	2.331443	-0.374666
12	6	-2.677389	0.531807	-2.041066
13	6	2.676596	0.534027	2.041053
14	8	-0.003670	-2.744184	-0.003465
15	1	-1.142366	3.458360	-1.923140
16	1	-1.658326	2.481491	-3.288446

17	1	0.388547	1.062842	-3.084225
18	1	0.853772	2.781034	-3.166531
19	1	1.025284	3.671904	-0.361997
20	1	2.362534	3.380066	-1.492282
21	1	3.330273	1.675351	-0.089720
22	1	3.145686	3.149311	0.864539
23	1	1.138547	3.459160	1.920761
24	1	1.656765	2.484435	3.286715
25	1	-0.387638	1.061459	3.083575
26	1	-0.855648	2.778875	3.166540
27	1	-1.025112	3.669168	0.360898
28	1	-2.362877	3.379249	1.491143
29	1	-3.331091	1.673776	0.089065
30	1	-3.146507	3.147805	-0.865033
31	1	-3.516172	1.008429	-2.570928
32	1	-2.061553	0.020322	-2.791188
33	1	3.514909	1.011343	2.571048
34	1	2.060636	0.022649	2.791135
35	1	-0.018277	-3.315134	0.781455
36	1	0.028165	-3.315272	-0.787842
37	8	1.008462	1.817525	-1.320417
38	8	-1.010234	1.815351	1.320477
39	6	-3.202923	-0.475359	-1.028842
40	6	-4.478513	-1.037679	-1.065195
41	6	-4.856414	-1.903695	-0.032554
42	1	-5.165065	-0.798407	-1.871289
43	6	-2.720093	-1.555528	0.989771
44	6	-3.976639	-2.158790	1.019986
45	1	-5.843694	-2.356318	-0.041908
46	1	-4.234267	-2.797752	1.856871
47	6	3.203093	-0.473570	1.029820
48	6	4.478936	-1.035280	1.067222
49	6	2.721675	-1.555927	-0.987971
50	6	4.857608	-1.902316	0.035727
51	1	5.165071	-0.794843	1.873323
52	6	3.978292	-2.159115	-1.016801
53	1	5.845068	-2.354529	0.045995
54	1	4.236383	-2.799325	-1.852595
55	7	2.355496	-0.763499	0.031391
56	7	-2.354712	-0.764065	-0.030593
57	6	-1.684369	-1.737428	2.104973
58	8	-0.614020	-0.996050	1.971921
59	8	-1.918003	-2.540114	2.995236
60	6	1.685885	-1.739775	-2.102821
61	8	1.916511	-2.549085	-2.987978
62	8	0.618575	-0.993552	-1.974300

E(RB3LYP) = -1638.4985438 Hartrees
Corrección de punto cero = 0.502753 Hartrees
Suma de las entalpías electrónicas y térmicas = -1637.963081 Hartrees
Suma de las energías libres y térmicas = -1638.057054 Hartrees

[Ho(dpa12c4)(H_2O)]$^+$ (vacío) **Δ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.000063	-0.000613	-0.177900
2	7	-1.392336	-1.784519	1.263032
3	6	-1.995088	-1.177373	2.483600

4	6	-2.288348	0.322255	2.379176
5	6	-0.823381	2.272782	2.356265
6	6	0.391218	2.834091	1.604154
7	7	1.391790	1.786815	1.259648
8	6	1.994881	1.181823	2.481139
9	6	2.288064	-0.318042	2.379414
10	6	0.823036	-2.268761	2.360057
11	6	-0.391832	-2.831310	1.609182
12	6	-2.423836	-2.341235	0.346774
13	6	2.422872	2.342477	0.342308
14	8	-0.005092	-0.005245	-2.703760
15	1	-1.292738	-1.314871	3.307297
16	1	-2.919775	-1.703812	2.762301
17	1	-3.152089	0.546157	1.745964
18	1	-2.494945	0.704371	3.386596
19	1	-0.643698	2.184510	3.436173
20	1	-1.671444	2.953173	2.210775
21	1	0.050470	3.259982	0.659538
22	1	0.834751	3.637768	2.212879
23	1	1.292774	1.320849	3.304788
24	1	2.919680	1.708685	2.758669
25	1	3.151692	-0.543134	1.746459
26	1	2.494843	-0.698309	3.387494
27	1	0.643623	-2.178697	3.439854
28	1	1.671030	-2.949417	2.215445
29	1	-0.051323	-3.259004	0.665293
30	1	-0.835286	-3.633829	2.219488
31	1	-1.903545	-2.966554	-0.388707
32	1	-3.127895	-2.991558	0.887015
33	1	1.902096	2.966118	-0.394242
34	1	3.126595	2.994197	0.881306
35	1	0.181812	-0.773951	-3.265395
36	1	-0.174586	0.766493	-3.266753
37	8	-1.129801	0.971102	1.841564
38	8	1.129432	-0.967889	1.843195
39	6	-3.168236	-1.241328	-0.388142
40	6	-4.518639	-1.302065	-0.732676
41	6	-5.080390	-0.226002	-1.428204
42	1	-5.118267	-2.165878	-0.462876
43	6	-2.957154	0.878921	-1.345898
44	6	-4.295973	0.886165	-1.735445
45	1	-6.128535	-0.252481	-1.711786
46	1	-4.686687	1.754722	-2.253164
47	6	3.167896	1.241717	-0.390582
48	6	4.518558	1.302142	-0.734143
49	6	2.958202	-0.880411	-1.344433
50	6	5.081158	0.225016	-1.427340
51	1	5.117768	2.166536	-0.465281
52	6	4.297299	-0.887956	-1.733056
53	1	6.129518	0.251269	-1.710146
54	1	4.688656	-1.757419	-2.248771
55	7	2.419843	0.175387	-0.711970
56	7	-2.419757	-0.175733	-0.710785
57	6	-2.026681	2.072007	-1.581575
58	8	-0.842351	1.936377	-1.045718
59	8	-2.443872	3.024042	-2.222829
60	6	2.028430	-2.074516	-1.577873
61	8	2.445928	-3.026993	-2.218328
62	8	0.844583	-1.939006	-1.041199

E(RB3LYP) = -1638.5083224 Hartrees
Corrección de punto cero = 0.503684 Hartrees
Suma de las entalpías electrónicas y térmicas = -1637.971973 Hartrees
Suma de las energías libres y térmicas = -1638.065741 Hartrees

$[Ho(dpa12c4)(H_2O)]^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.000003	-0.090672	-0.000018
2	7	1.597829	1.209987	1.648141
3	6	0.713021	1.755361	2.708582
4	6	-0.398819	2.654113	2.171138
5	6	-1.758751	2.955617	0.221818
6	6	-2.428823	2.224495	-0.943393
7	7	-1.597872	1.209943	-1.648163
8	6	-0.713071	1.755293	-2.708625
9	6	0.398775	2.654058	-2.171207
10	6	1.758708	2.955617	-0.221886
11	6	2.428779	2.224522	0.943343
12	6	2.493667	0.159990	2.221806
13	6	-2.493712	0.159920	-2.221776
14	8	-0.000259	-2.664298	-0.000152
15	1	1.285718	2.329566	3.454647
16	1	0.259531	0.895553	3.205987
17	1	-1.088044	3.753336	-0.117894
18	1	-2.545502	3.428397	0.825029
19	1	-3.298836	1.701889	-0.542995
20	1	-2.806601	2.979221	-1.650820
21	1	-1.285771	2.329486	-3.454697
22	1	-0.259585	0.895477	-3.206016
23	1	1.088001	3.753345	0.117805
24	1	2.545461	3.428382	-0.825107
25	1	3.298792	1.701906	0.542959
26	1	2.806558	2.979268	1.650750
27	1	3.256790	0.598991	2.881139
28	1	1.867580	-0.502298	2.830206
29	1	-3.256854	0.598892	-2.881107
30	1	-1.867639	-0.502384	-2.830173
31	1	0.091591	-3.230783	-0.782229
32	1	-0.091038	-3.230927	0.781946
33	8	-1.018290	2.035448	1.029276
34	8	1.018248	2.035429	-1.029324
35	6	3.141328	-0.638078	1.103093
36	6	4.430699	-1.168281	1.140351
37	6	4.894619	-1.870542	0.021781
38	1	5.059566	-1.032695	2.014810
39	6	2.802672	-1.448720	-1.063270
40	6	4.079066	-2.008657	-1.102381
41	1	5.895070	-2.293369	0.026684
42	1	4.399738	-2.527257	-1.998677
43	6	-3.141336	-0.638121	-1.103020
44	6	-4.430677	-1.168400	-1.140255
45	6	-2.802617	-1.448675	1.063364
46	6	-4.894550	-1.870641	-0.021656
47	1	-5.059554	-1.032886	-2.014718
48	6	-4.078983	-2.008673	1.102506
49	1	-5.894979	-2.293521	-0.026534
50	1	-4.399623	-2.527256	1.998824

51	7	-2.362841	-0.798766	-0.023753
52	7	2.362843	-0.798809	0.023828
53	6	1.817247	-1.531063	-2.231776
54	8	0.679333	-0.924158	-2.010171
55	8	2.145261	-2.140819	-3.237482
56	6	-1.817183	-1.530934	2.231864
57	8	-2.145119	-2.140748	3.237557
58	8	-0.679190	-0.924203	2.010139
59	1	1.148358	2.808024	-2.957282
60	1	0.016950	3.639815	-1.878332
61	1	-0.016989	3.639860	1.878235
62	1	-1.148401	2.808107	2.957208

E(RB3LYP) = -1638.5089639 Hartrees
Corrección de punto cero = 0.503735 Hartrees
Suma de las entalpías electrónicas y térmicas = -1637.972555 Hartrees
Suma de las energías libres y térmicas = -1638.066523 Hartrees

[Yb(dpa12c4)(H_2O)]$^+$ (vacío) Λ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	70	-0.030474	0.082067	-0.083401
2	7	2.016033	1.429674	1.037075
3	6	1.538526	2.258659	2.180343
4	6	0.209767	1.754331	2.739397
5	6	-1.595879	2.735105	1.372619
6	6	-2.628942	2.293773	0.339588
7	7	-2.012867	1.716516	-0.886571
8	6	-1.498628	2.781919	-1.790105
9	6	-0.189657	2.362130	-2.453973
10	6	1.610461	2.982125	-0.895723
11	6	2.636554	2.282242	-0.014027
12	6	2.984441	0.376171	1.470155
13	6	-2.976656	0.829394	-1.597448
14	8	1.301304	-1.132470	3.715162
15	1	1.420005	3.288567	1.829462
16	1	2.282070	2.285202	2.988646
17	1	0.319087	0.764178	3.191742
18	1	-0.180947	2.444767	3.495185
19	1	-0.985302	3.575451	1.014877
20	1	-2.113601	3.059507	2.283469
21	1	-3.254965	1.525083	0.796588
22	1	-3.279794	3.146479	0.093688
23	1	-1.328208	3.685968	-1.198065
24	1	-2.240192	3.045959	-2.557500
25	1	-0.318311	1.479960	-3.086301
26	1	0.222276	3.174245	-3.063499
27	1	1.010874	3.714490	-0.337964
28	1	2.126079	3.512766	-1.705410
29	1	3.243445	1.639852	-0.655038
30	1	3.306869	3.033541	0.430014
31	1	3.944993	0.829091	1.759546
32	1	2.576520	-0.127318	2.357381
33	1	-3.905900	1.367796	-1.837305
34	1	-2.513984	0.532546	-2.545994
35	1	1.292535	-1.757869	4.455385
36	1	0.772188	-1.558142	3.006699
37	8	-0.763245	1.607476	1.671888

38	8	0.766401	1.964881	-1.451053
39	6	3.201862	-0.640927	0.362590
40	6	4.389535	-1.350336	0.179457
41	6	4.475549	-2.255278	-0.883030
42	1	5.230075	-1.196119	0.848843
43	6	2.245626	-1.666315	-1.513047
44	6	3.397464	-2.409381	-1.756187
45	1	5.389800	-2.820654	-1.038257
46	1	3.425957	-3.072855	-2.612878
47	6	-3.280608	-0.419616	-0.790951
48	6	-4.497110	-1.100249	-0.845033
49	6	-2.438629	-1.937005	0.767040
50	6	-4.658512	-2.248548	-0.063809
51	1	-5.300600	-0.742005	-1.481041
52	6	-3.621404	-2.672048	0.768008
53	1	-5.595082	-2.797255	-0.094644
54	1	-3.704775	-3.539689	1.412381
55	7	-2.283123	-0.849893	-0.006296
56	7	2.161719	-0.827110	-0.465451
57	6	1.019636	-1.705623	-2.425126
58	8	0.023354	-0.960552	-1.993183
59	8	1.048004	-2.372205	-3.441834
60	6	-1.254168	-2.269793	1.658977
61	8	-1.339894	-3.141902	2.504159
62	8	-0.197880	-1.516092	1.429670

E(RB3LYP) = -1640.2615886 Hartrees
Corrección de punto cero = 0.503872 Hartrees
Suma de las entalpías electrónicas y térmicas = -1639.725477 Hartrees
Suma de las energías libres y térmicas = -1639.817525 Hartrees

[Yb(dpa12c4)(H_2O)]$^+$ (vacío) **Δ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	70	0.000002	-0.000009	-0.150839
2	7	1.382280	1.783472	1.255079
3	6	2.000366	1.183327	2.471078
4	6	2.292345	-0.315779	2.366708
5	6	0.825694	-2.261920	2.360239
6	6	-0.388713	-2.830876	1.614588
7	7	-1.382213	-1.782692	1.256186
8	6	-2.000333	-1.181819	2.471809
9	6	-2.292243	0.317237	2.366551
10	6	-0.825642	2.263416	2.358806
11	6	0.388804	2.831900	1.612833
12	6	2.400946	2.336517	0.323023
13	6	-2.400848	-2.336363	0.324464
14	8	0.000274	-0.000627	-2.669108
15	1	1.306696	1.322810	3.301977
16	1	2.927165	1.712228	2.737719
17	1	3.151991	-0.541546	1.728587
18	1	2.503887	-0.698411	3.372757
19	1	0.647456	-2.164762	3.439622
20	1	1.675879	-2.940532	2.219294
21	1	-0.049103	-3.269858	0.676387
22	1	-0.837397	-3.623491	2.233811
23	1	-1.306712	-1.320860	3.302824
24	1	-2.927167	-1.710527	2.738703

25	1	-3.151858	0.542663	1.728262
26	1	-2.503802	0.700475	3.372365
27	1	-0.647476	2.167055	3.438271
28	1	-1.675854	2.941877	2.217303
29	1	0.049226	3.270336	0.674367
30	1	0.837499	3.624866	2.231596
31	1	1.869843	2.957313	-0.408140
32	1	3.114003	2.987562	0.850225
33	1	-1.869699	-2.957556	-0.406327
34	1	-3.113858	-2.987138	0.852060
35	1	-0.144643	0.775958	-3.232159
36	1	0.144043	-0.777738	-3.231723
37	8	1.129400	-0.962774	1.835904
38	8	-1.129245	0.963863	1.835407
39	6	3.130224	1.230605	-0.416392
40	6	4.473558	1.284584	-0.788914
41	6	5.019301	0.199821	-1.483339
42	1	5.079886	2.150104	-0.540489
43	6	2.895878	-0.898402	-1.348196
44	6	4.226569	-0.914025	-1.762953
45	1	6.061747	0.220717	-1.787612
46	1	4.605347	-1.789310	-2.278219
47	6	-3.130202	-1.230945	-0.415608
48	6	-4.473553	-1.285202	-0.788029
49	6	-2.895988	0.897503	-1.348717
50	6	-5.019371	-0.200892	-1.483102
51	1	-5.079837	-2.150589	-0.539033
52	6	-4.226696	0.912815	-1.763430
53	1	-6.061831	-0.222016	-1.787311
54	1	-4.605535	1.787778	-2.279202
55	7	-2.373374	-0.164338	-0.713218
56	7	2.373348	0.163837	-0.713301
57	6	1.954066	-2.086402	-1.553623
58	8	0.777890	-1.930720	-1.004884
59	8	2.352926	-3.052967	-2.184639
60	6	-1.954250	2.085445	-1.554823
61	8	-2.353119	3.051557	-2.186530
62	8	-0.778100	1.930167	-1.005933

E(RB3LYP) = -1640.2584774 Hartrees
Corrección de punto cero = 0.503988 Hartrees
Suma de las entalpías electrónicas y térmicas = -1639.721861 Hartrees
Suma de las energías libres y térmicas = -1639.815692 Hartrees

[Yb(dpa12c4)(H_2O)]$^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	70	-0.000856	-0.071325	-0.004953
2	7	-1.591551	1.203686	-1.643422
3	6	-0.716126	1.760245	-2.704964
4	6	0.398710	2.651302	-2.161310
5	6	1.753263	2.945272	-0.209872
6	6	2.421070	2.210227	0.953015
7	7	1.582452	1.196979	1.649936
8	6	0.704083	1.744308	2.714076
9	6	-0.412410	2.635982	2.176177
10	6	-1.766813	2.939033	0.227551
11	6	-2.432562	2.210702	-0.940397

12	6	-2.477142	0.143772	-2.213602
13	6	2.469808	0.138165	2.219142
14	8	-0.042787	-2.649522	-0.023032
15	1	-1.294438	2.344152	-3.438927
16	1	-0.267107	0.906515	-3.215218
17	1	1.082858	3.742624	0.131482
18	1	2.539564	3.418435	-0.813172
19	1	3.290518	1.686605	0.552513
20	1	2.799454	2.960924	1.664187
21	1	1.280320	2.323841	3.453088
22	1	0.256700	0.885476	3.217204
23	1	-1.098322	3.740469	-0.108122
24	1	-2.554138	3.405874	0.834419
25	1	-3.301426	1.683042	-0.544223
26	1	-2.811368	2.965352	-1.647110
27	1	-3.248782	0.572971	-2.869258
28	1	-1.845193	-0.512812	-2.821546
29	1	3.238206	0.567737	2.878383
30	1	1.837592	-0.521938	2.822825
31	1	0.030893	-3.192915	0.777280
32	1	0.141955	-3.212729	-0.791064
33	8	1.011815	2.026481	-1.018500
34	8	-1.022702	2.016492	1.029504
35	6	-3.106724	-0.657679	-1.088134
36	6	-4.386515	-1.211381	-1.114405
37	6	-4.831897	-1.913266	0.011611
38	1	-5.021987	-1.093456	-1.986626
39	6	-2.740409	-1.450758	1.079223
40	6	-4.006907	-2.030219	1.131473
41	1	-5.824927	-2.353237	0.015691
42	1	-4.312993	-2.548599	2.032977
43	6	3.106212	-0.657481	1.093887
44	6	4.390970	-1.199902	1.120055
45	6	2.753697	-1.439860	-1.080079
46	6	4.845190	-1.893030	-0.007893
47	1	5.023960	-1.079053	1.993683
48	6	4.024646	-2.010081	-1.131129
49	1	5.842023	-2.324329	-0.011509
50	1	4.338117	-2.519533	-2.035234
51	7	2.321602	-0.799992	0.016504
52	7	-2.319144	-0.797382	-0.013072
53	6	-1.741502	-1.514118	2.234374
54	8	-0.606950	-0.908532	1.985374
55	8	-2.050811	-2.105513	3.256271
56	6	1.761119	-1.495901	-2.242361
57	8	2.071835	-2.098330	-3.257893
58	8	0.634266	-0.875906	-2.003074
59	1	-1.166975	2.782703	2.958800
60	1	-0.037246	3.625409	1.886883
61	1	0.020690	3.637538	-1.865020
62	1	1.152583	2.805309	-2.943135

E(RB3LYP) = -1640.2591105 Hartrees
Corrección de punto cero = 0.504213 Hartrees
Suma de las entalpías electrónicas y térmicas = -1639.722445 Hartrees
Suma de las energías libres y térmicas = -1639.814731 Hartrees

[Lu(dpa12c4)(H_2O)]$^+$ (vacío) Λ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.031030	0.089466	-0.082646
2	7	2.014066	1.420930	1.037808
3	6	1.540470	2.242951	2.187585
4	6	0.212354	1.735655	2.744932
5	6	-1.595865	2.722134	1.386400
6	6	-2.629523	2.285054	0.352501
7	7	-2.012739	1.712910	-0.875574
8	6	-1.503423	2.782251	-1.777176
9	6	-0.194795	2.366671	-2.443838
10	6	1.606499	2.982419	-0.885782
11	6	2.634073	2.279561	-0.008660
12	6	2.982381	0.363418	1.460710
13	6	-2.974322	0.823820	-1.586988
14	8	1.321515	-1.148593	3.718881
15	1	1.421889	3.275177	1.843570
16	1	2.285704	2.263452	2.994435
17	1	0.322051	0.743789	3.192891
18	1	-0.178940	2.422565	3.503550
19	1	-0.987686	3.566131	1.033256
20	1	-2.112101	3.038816	2.300725
21	1	-3.254864	1.514153	0.806613
22	1	-3.280915	3.138289	0.110117
23	1	-1.333995	3.685011	-1.182829
24	1	-2.247198	3.046459	-2.542339
25	1	-0.322801	1.486896	-3.079316
26	1	0.216805	3.181758	-3.049502
27	1	1.008039	3.713034	-0.324545
28	1	2.119962	3.515256	-1.695329
29	1	3.241181	1.641053	-0.653316
30	1	3.303986	3.028788	0.439325
31	1	3.945918	0.812834	1.745599
32	1	2.579686	-0.142615	2.348749
33	1	-3.906368	1.358803	-1.823408
34	1	-2.512043	0.530253	-2.536628
35	1	1.313085	-1.782485	4.451874
36	1	0.795973	-1.568474	3.004856
37	8	-0.760097	1.593948	1.675985
38	8	0.761443	1.966216	-1.441838
39	6	3.189236	-0.648290	0.346421
40	6	4.371082	-1.365193	0.154588
41	6	4.447043	-2.263565	-0.914126
42	1	5.214824	-1.221587	0.822307
43	6	2.219251	-1.654892	-1.532025
44	6	3.364780	-2.404366	-1.784482
45	1	5.356643	-2.834491	-1.076193
46	1	3.385548	-3.062619	-2.645424
47	6	-3.269427	-0.427556	-0.781451
48	6	-4.481023	-1.117052	-0.833298
49	6	-2.412788	-1.940334	0.772667
50	6	-4.632332	-2.266983	-0.052484
51	1	-5.288446	-0.764325	-1.467405
52	6	-3.590062	-2.684019	0.776248
53	1	-5.565030	-2.822342	-0.081522
54	1	-3.665497	-3.553133	1.419621
55	7	-2.267305	-0.851032	0.000768

56	7	2.145119	-0.821397	-0.479211
57	6	0.988220	-1.679678	-2.436942
58	8	-0.001009	-0.932787	-1.991514
59	8	1.005512	-2.337260	-3.459667
60	6	-1.221224	-2.264787	1.657349
61	8	-1.294327	-3.137244	2.503546
62	8	-0.171775	-1.503745	1.420696

E(RB3LYP) = -1640.8183037 Hartrees
Corrección de punto cero = 0.503950 Hartrees
Suma de las entalpías electrónicas y térmicas = -1640.282135 Hartrees
Suma de las energías libres y térmicas = -1640.374101 Hartrees

[Lu(dpa12c4)(H_2O)]$^+$ (vacío) **Δ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.000133	-0.000358	-0.141739
2	7	-1.381383	-1.779299	1.257416
3	6	-2.003563	-1.178765	2.470893
4	6	-2.294830	0.319917	2.362978
5	6	-0.823475	2.261517	2.360826
6	6	0.390899	2.830859	1.616128
7	7	1.381254	1.781251	1.254498
8	6	2.003763	1.182480	2.468680
9	6	2.295043	-0.316381	2.362928
10	6	0.823610	-2.258044	2.363905
11	6	-0.391002	-2.828431	1.620347
12	6	-2.396839	-2.331664	0.321628
13	6	2.396313	2.332533	0.317687
14	8	-0.004387	-0.003390	-2.660829
15	1	-1.312333	-1.317166	3.304073
16	1	-2.930975	-1.707730	2.735254
17	1	-3.153597	0.544696	1.723401
18	1	-2.507077	0.705398	3.367712
19	1	-0.644096	2.159251	3.439523
20	1	-1.672650	2.942140	2.223883
21	1	0.051582	3.272935	0.679504
22	1	0.841813	3.620621	2.237365
23	1	1.312727	1.322071	3.301819
24	1	2.931236	1.711824	2.732098
25	1	3.153731	-0.542096	1.723562
26	1	2.507477	-0.700357	3.368197
27	1	0.644478	-2.154120	3.442481
28	1	1.672689	-2.938947	2.227790
29	1	-0.051940	-3.271961	0.684318
30	1	-0.841774	-3.617239	2.242896
31	1	-1.863444	-2.953594	-0.406759
32	1	-3.113743	-2.980584	0.846168
33	1	1.862508	2.953108	-0.411540
34	1	3.113101	2.982529	0.841056
35	1	0.133826	-0.781292	-3.223589
36	1	-0.124222	0.777311	-3.223926
37	8	-1.130859	0.964948	1.831559
38	8	1.131046	-0.962272	1.832640
39	6	-3.119429	-1.224401	-0.421767
40	6	-4.460338	-1.275034	-0.803514
41	6	-4.998917	-0.188582	-1.500771
42	1	-5.070249	-2.139380	-0.559830

43	6	-2.873846	0.904119	-1.351473
44	6	-4.201660	0.923506	-1.774752
45	1	-6.039363	-0.206856	-1.811979
46	1	-4.574845	1.799778	-2.292417
47	6	3.119198	1.224393	-0.424041
48	6	4.460356	1.274459	-0.804991
49	6	2.874371	-0.905641	-1.350457
50	6	4.999455	0.186991	-1.500267
51	1	5.070091	2.139158	-0.562122
52	6	4.202444	-0.925584	-1.772950
53	1	6.040106	0.204838	-1.810814
54	1	4.576013	-1.802708	-2.288900
55	7	2.358122	0.158844	-0.714256
56	7	-2.358211	-0.159302	-0.713055
57	6	-1.925848	2.087435	-1.551577
58	8	-0.753850	1.925976	-0.995371
59	8	-2.315030	3.055503	-2.186281
60	6	1.926733	-2.089618	-1.548689
61	8	2.316111	-3.058196	-2.182552
62	8	0.755135	-1.927952	-0.991977

E(RB3LYP) = -1640.8145574 Hartrees
Corrección de punto cero = 0.504128 Hartrees
Suma de las entalpías electrónicas y térmicas = -1640.277840 Hartrees
Suma de las energías libres y térmicas = -1640.371517 Hartrees

[Lu(dpa12c4)(H_2O)]$^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.000794	-0.063300	-0.004521
2	7	-1.592268	1.201425	-1.640100
3	6	-0.721756	1.759483	-2.704683
4	6	0.395330	2.648845	-2.163530
5	6	1.754597	2.943042	-0.216784
6	6	2.423876	2.209057	0.945413
7	7	1.583905	1.198454	1.644248
8	6	0.710459	1.749273	2.710389
9	6	-0.408507	2.637940	2.173182
10	6	-1.767867	2.936871	0.228600
11	6	-2.434878	2.207037	-0.937215
12	6	-2.476230	0.138652	-2.207080
13	6	2.469929	0.137903	2.211806
14	8	-0.038334	-2.647088	-0.018550
15	1	-1.303210	2.344816	-3.434994
16	1	-0.275286	0.906568	-3.218107
17	1	1.085734	3.741589	0.124878
18	1	2.539510	3.414160	-0.823419
19	1	3.291742	1.683451	0.544047
20	1	2.804767	2.959855	1.655100
21	1	1.289750	2.331981	3.444489
22	1	0.265817	0.892269	3.218621
23	1	-1.101106	3.738975	-0.108978
24	1	-2.553954	3.402714	0.837770
25	1	-3.302037	1.677994	-0.539116
26	1	-2.816367	2.960248	-1.643977
27	1	-3.251963	0.565057	-2.859692
28	1	-1.844161	-0.516247	-2.816458
29	1	3.242778	0.565918	2.866814

30	1	1.837963	-0.519448	2.818491
31	1	0.041821	-3.193038	0.779257
32	1	0.119829	-3.212841	-0.790527
33	8	1.009873	2.023279	-1.021637
34	8	-1.020306	2.015225	1.028743
35	6	-3.097692	-0.663798	-1.078404
36	6	-4.374600	-1.224477	-1.098651
37	6	-4.812097	-1.926457	0.030291
38	1	-5.013878	-1.111576	-1.968745
39	6	-2.718951	-1.451275	1.088455
40	6	-3.982057	-2.037106	1.147112
41	1	-5.802797	-2.371585	0.039005
42	1	-4.281623	-2.555757	2.050652
43	6	3.097588	-0.660988	1.084486
44	6	4.379133	-1.211317	1.105514
45	6	2.731360	-1.442622	-1.087015
46	6	4.824671	-1.907370	-0.023976
47	1	5.016184	-1.094192	1.976686
48	6	3.998551	-2.020214	-1.143611
49	1	5.818889	-2.344612	-0.031575
50	1	4.304785	-2.532481	-2.048605
51	7	2.307662	-0.798805	0.010494
52	7	-2.305134	-0.797136	-0.006240
53	6	-1.713294	-1.508540	2.237175
54	8	-0.584518	-0.895423	1.980263
55	8	-2.010927	-2.102600	3.260938
56	6	1.731236	-1.495776	-2.241959
57	8	2.029473	-2.103350	-3.258103
58	8	0.609894	-0.868321	-1.995557
59	1	-1.161986	2.785344	2.956675
60	1	-0.035527	3.627263	1.880708
61	1	0.019350	3.635561	-1.866219
62	1	1.148173	2.802008	-2.946476

E(RB3LYP) = -1640.8150815 Hartrees
Corrección de punto cero = 0.504260 Hartrees
Suma de las entalpías electrónicas y térmicas = -1640.278361 Hartrees
Suma de las energías libres y térmicas = -1640.370713 Hartrees

$[La(dpa12c4)(H_2O)_2]^+$ (vacío) Δ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.000194	-0.000314	-0.426785
2	7	1.380879	1.818664	1.301467
3	6	1.843764	1.188013	2.567364
4	6	2.209098	-0.297700	2.467506
5	6	0.895288	-2.332525	2.254966
6	6	-0.352801	-2.866442	1.536869
7	7	-1.381764	-1.819307	1.300789
8	6	-1.845203	-1.189011	2.566623
9	6	-2.210021	0.296856	2.467151
10	6	-0.896540	2.331739	2.254919
11	6	0.351885	2.865814	1.537470
12	6	2.508832	2.380730	0.519415
13	6	-2.509389	-2.380893	0.517985
14	8	-0.922498	-1.556999	-2.434489
15	1	1.041224	1.271640	3.300071
16	1	2.708584	1.732135	2.977607

17	1	3.144440	-0.472617	1.929452
18	1	2.328873	-0.682210	3.489027
19	1	0.767065	-2.326388	3.345730
20	1	1.746761	-2.984313	2.021816
21	1	-0.061696	-3.252305	0.555258
22	1	-0.750417	-3.711971	2.121469
23	1	-1.043153	-1.273166	3.299811
24	1	-2.710424	-1.733036	2.976146
25	1	-3.145132	0.472284	1.928842
26	1	-2.330064	0.680997	3.488795
27	1	-0.769068	2.326101	3.345782
28	1	-1.748097	2.983103	2.020894
29	1	0.061170	3.251930	0.555859
30	1	0.749403	3.711100	2.122474
31	1	2.081178	2.970988	-0.300047
32	1	3.114493	3.065639	1.133273
33	1	-2.081490	-2.970908	-0.301524
34	1	-3.115469	-3.065942	1.131284
35	1	-1.293173	-1.443899	-3.322410
36	1	-0.068002	-2.046608	-2.496703
37	8	1.142410	-0.995210	1.814226
38	8	-1.142835	0.994156	1.814595
39	6	3.383147	1.297069	-0.081230
40	6	4.769875	1.412733	-0.188340
41	6	5.486455	0.370751	-0.784517
42	1	5.278209	2.295567	0.187455
43	6	3.416414	-0.797608	-1.087451
44	6	4.804208	-0.756757	-1.237366
45	1	6.566126	0.437887	-0.881986
46	1	5.305041	-1.602060	-1.695176
47	6	-3.383265	-1.296737	-0.082498
48	6	-4.769997	-1.411930	-0.189919
49	6	-3.415723	0.798481	-1.087625
50	6	-5.486168	-0.369440	-0.785724
51	1	-5.278666	-2.294795	0.185352
52	6	-4.803510	0.758093	-1.237866
53	1	-6.565837	-0.436229	-0.883438
54	1	-5.303992	1.603772	-1.695365
55	7	-2.731597	-0.213833	-0.532722
56	7	2.731886	0.214230	-0.532121
57	6	2.605616	-2.006850	-1.545241
58	8	1.318219	-1.896783	-1.334659
59	8	3.184345	-2.951185	-2.058173
60	6	-2.604515	2.007773	-1.544505
61	8	-3.182818	2.952273	-2.057619
62	8	-1.317275	1.897638	-1.332932
63	8	0.922788	1.557195	-2.434061
64	1	0.068475	2.047159	-2.495898
65	1	1.293397	1.444127	-3.322011

E(RB3LYP) = -1708.854633 Hartrees
Corrección de punto cero = 0.528407 Hartrees
Suma de las entalpías electrónicas y térmicas = -1708.291043 Hartrees
Suma de las energías libres y térmicas = -1708.389907 Hartrees

$[La(dpa12c4)(H_2O)_2]^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z

1	57	0.038987	-0.265408	-0.161350
2	7	-1.893713	1.130429	-1.674354
3	6	-1.038360	1.613207	-2.783955
4	6	0.063746	2.586720	-2.347263
5	6	1.418821	3.097232	-0.419629
6	6	2.151829	2.513562	0.798525
7	7	1.448579	1.469401	1.592852
8	6	0.491771	1.977274	2.608358
9	6	-0.648405	2.804206	2.039237
10	6	-2.012298	2.974560	0.109825
11	6	-2.697169	2.184896	-1.000745
12	6	-2.841058	0.068114	-2.128533
13	6	2.449720	0.625363	2.309074
14	8	-0.831400	-2.172482	-1.961676
15	1	-1.627351	2.117507	-3.568375
16	1	-0.576293	0.733466	-3.246359
17	1	0.679016	3.849526	-0.129111
18	1	2.169238	3.603130	-1.041670
19	1	3.075780	2.063042	0.434639
20	1	2.444097	3.362966	1.437867
21	1	1.006960	2.589286	3.367625
22	1	0.076561	1.098094	3.109983
23	1	-1.368110	3.771129	-0.282126
24	1	-2.795722	3.464704	0.705321
25	1	-3.557237	1.684680	-0.553655
26	1	-3.095305	2.898699	-1.739916
27	1	-3.655175	0.496348	-2.732285
28	1	-2.293776	-0.641035	-2.754625
29	1	3.064228	1.232220	2.992149
30	1	1.884801	-0.082562	2.927998
31	1	-0.820954	-3.013423	-1.473553
32	1	0.066114	-2.094624	-2.373076
33	8	0.764027	2.081683	-1.193252
34	8	-1.240107	2.108562	0.937614
35	6	-3.407496	-0.665931	-0.921066
36	6	-4.729040	-1.103334	-0.830738
37	6	-5.151560	-1.728461	0.347771
38	1	-5.416829	-0.950786	-1.656943
39	6	-2.951587	-1.420028	1.240703
40	6	-4.260493	-1.875407	1.409602
41	1	-6.176023	-2.077458	0.438938
42	1	-4.544292	-2.321214	2.355936
43	6	3.336289	-0.134410	1.344143
44	6	4.685006	-0.401313	1.583329
45	6	3.436762	-1.154791	-0.744007
46	6	5.412293	-1.094475	0.610722
47	1	5.157465	-0.069509	2.502834
48	6	4.786288	-1.469018	-0.577338
49	1	6.462395	-1.318775	0.773892
50	1	5.305048	-1.984047	-1.377844
51	7	2.732697	-0.526582	0.212163
52	7	-2.548067	-0.851580	0.094970
53	6	-1.913250	-1.519760	2.360120
54	8	-0.695918	-1.167789	2.007412
55	8	-2.266289	-1.909457	3.460021
56	6	2.685459	-1.496114	-2.027310
57	8	3.252318	-2.146724	-2.890863
58	8	1.459318	-1.043502	-2.055358
59	1	-1.397158	2.970818	2.825117
60	1	-0.299019	3.790259	1.706001

61	1	-0.354613	3.570692	-2.106979
62	1	0.770336	2.716031	-3.175905
63	8	0.577568	-2.885110	0.495689
64	1	0.246841	-2.719023	1.405730
65	1	1.410493	-3.377561	0.564244

E(RB3LYP) = -1708.8511097 Hartrees
Corrección de punto cero = 0.528936 Hartrees
Suma de las entalpías electrónicas y térmicas = -1708.287257 Hartrees
Suma de las energías libres y térmicas = -1708.385414 Hartrees

$[Nd(dpa12c4)(H_2O)_2]^+$ (vacío) **Δ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	60	0.000021	-0.000105	-0.391769
2	7	-1.332423	-1.840270	1.260362
3	6	-1.813842	-1.235061	2.533233
4	6	-2.196290	0.247275	2.453899
5	6	-0.948819	2.317229	2.209567
6	6	0.292022	2.876452	1.495752
7	7	1.332192	1.840576	1.260026
8	6	1.813577	1.235642	2.533044
9	6	2.196002	-0.246726	2.454072
10	6	0.948541	-2.316756	2.210103
11	6	-0.292299	-2.876123	1.496376
12	6	-2.448522	-2.406292	0.464511
13	6	2.448282	2.406528	0.464118
14	8	0.915741	1.461016	-2.424606
15	1	-1.016121	-1.322717	3.270641
16	1	-2.674886	-1.796968	2.926348
17	1	-3.139273	0.418429	1.927537
18	1	-2.309325	0.620291	3.480592
19	1	-0.836347	2.339292	3.301913
20	1	-1.820077	2.931189	1.949274
21	1	-0.002719	3.258017	0.514814
22	1	0.679996	3.722563	2.085438
23	1	1.015846	1.323496	3.270419
24	1	2.674628	1.797618	2.926046
25	1	3.139010	-0.418014	1.927798
26	1	2.308976	-0.619502	3.480858
27	1	0.836047	-2.338600	3.302451
28	1	1.819802	-2.930766	1.949945
29	1	0.002468	-3.257956	0.515551
30	1	-0.680315	-3.722075	2.086262
31	1	-2.009830	-2.978510	-0.361625
32	1	-3.050289	-3.106123	1.064914
33	1	2.009567	2.978522	-0.362168
34	1	3.049930	3.106575	1.064389
35	1	1.253919	1.299596	-3.318063
36	1	0.080959	1.981907	-2.478101
37	8	-1.142573	0.960755	1.798950
38	8	1.142316	-0.960356	1.799231
39	6	-3.326025	-1.318069	-0.121137
40	6	-4.709804	-1.439593	-0.256573
41	6	-5.423228	-0.383303	-0.831051
42	1	-5.218412	-2.337239	0.081920
43	6	-3.357220	0.807244	-1.059571
44	6	-4.741682	0.763688	-1.234474

45	1	-6.500554	-0.454294	-0.949395
46	1	-5.241373	1.620657	-1.671486
47	6	3.325955	1.318282	-0.121225
48	6	4.709725	1.439952	-0.256618
49	6	3.357457	-0.807230	-1.059186
50	6	5.423308	0.383628	-0.830835
51	1	5.218203	2.337735	0.081703
52	6	4.741920	-0.763531	-1.234046
53	1	6.500631	0.454726	-0.949143
54	1	5.241735	-1.620529	-1.670862
55	7	2.676031	0.217501	-0.525891
56	7	-2.675952	-0.217457	-0.526024
57	6	-2.539286	2.030255	-1.458096
58	8	-1.253470	1.902234	-1.241790
59	8	-3.106361	3.000754	-1.933542
60	6	2.539706	-2.030435	-1.457490
61	8	3.106903	-3.000882	-1.932892
62	8	1.253896	-1.902615	-1.241043
63	8	-0.915881	-1.463020	-2.423512
64	1	-0.080746	-1.983460	-2.476435
65	1	-1.253100	-1.301426	-3.317305

E(RB3LYP) = -1710.762959 Hartrees
Corrección de punto cero = 0.528506 Hartrees
Suma de las entalpías electrónicas y térmicas = -1710.199275 Hartrees
Suma de las energías libres y térmicas = -1710.298229 Hartrees

[Nd(dpa12c4)(H_2O)$_2$]$^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	60	0.031763	-0.233689	-0.161497
2	7	-1.815983	1.184051	-1.653880
3	6	-0.931368	1.706605	-2.722718
4	6	0.159246	2.652006	-2.205121
5	6	1.444811	3.068904	-0.208321
6	6	2.133718	2.419571	1.001735
7	7	1.399017	1.329443	1.702109
8	6	0.429726	1.784187	2.730195
9	6	-0.693264	2.646790	2.179494
10	6	-1.980593	2.940183	0.211552
11	6	-2.632518	2.219093	-0.963291
12	6	-2.757824	0.142975	-2.163959
13	6	2.372748	0.418367	2.372868
14	8	-0.822677	-2.121511	-1.945740
15	1	-1.498503	2.248659	-3.497525
16	1	-0.458191	0.845507	-3.206347
17	1	0.706435	3.818220	0.094614
18	1	2.217585	3.591131	-0.787974
19	1	3.073447	1.993856	0.649534
20	1	2.395115	3.228472	1.702966
21	1	0.935251	2.351989	3.529032
22	1	0.002113	0.881368	3.174389
23	1	-1.314017	3.747514	-0.114778
24	1	-2.778926	3.407553	0.805294
25	1	-3.519036	1.714694	-0.577238
26	1	-2.986256	2.974088	-1.683175
27	1	-3.559421	0.594631	-2.767050
28	1	-2.202771	-0.547476	-2.803361

29	1	2.985799	0.962021	3.108113
30	1	1.784137	-0.324116	2.924821
31	1	-0.704593	-2.942281	-1.436065
32	1	0.038143	-1.980255	-2.408318
33	8	0.800966	2.094792	-1.040749
34	8	-1.248297	2.020313	1.017882
35	6	-3.343978	-0.625224	-0.988320
36	6	-4.663715	-1.073073	-0.930177
37	6	-5.101047	-1.729553	0.225713
38	1	-5.338908	-0.905210	-1.763720
39	6	-2.917414	-1.433536	1.158832
40	6	-4.225583	-1.899888	1.297266
41	1	-6.124719	-2.086343	0.291863
42	1	-4.521425	-2.372914	2.226596
43	6	3.258925	-0.274294	1.358794
44	6	4.599551	-0.591311	1.581838
45	6	3.363308	-1.080126	-0.821703
46	6	5.324181	-1.195894	0.549442
47	1	5.068737	-0.362436	2.533819
48	6	4.705844	-1.431998	-0.678132
49	1	6.368173	-1.455864	0.698259
50	1	5.226245	-1.866262	-1.524203
51	7	2.661170	-0.542592	0.188612
52	7	-2.500908	-0.829717	0.036923
53	6	-1.886802	-1.560768	2.278880
54	8	-0.664320	-1.215979	1.929180
55	8	-2.240496	-1.961072	3.374091
56	6	2.613552	-1.262661	-2.136694
57	8	3.185087	-1.782857	-3.081108
58	8	1.379720	-0.828444	-2.100375
59	1	-1.468105	2.766144	2.948196
60	1	-0.334298	3.650528	1.917114
61	1	-0.260022	3.630523	-1.943722
62	1	0.904127	2.804441	-2.995120
63	8	0.600273	-2.872164	0.369283
64	1	0.250823	-2.715357	1.275076
65	1	1.453128	-3.326529	0.453601

E(RB3LYP) = -1710.7602199 Hartrees
Corrección de punto cero = 0.529756 Hartrees
Suma de las entalpías electrónicas y térmicas = -1710.195889 Hartrees
Suma de las energías libres y térmicas = -1710.292726 Hartrees

$[Gd(dpa12c4)(H_2O)_2]^+$ (vacío) Δ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.015753	-0.153999	-0.287419
2	7	1.201907	1.985646	1.086605
3	6	1.707867	1.530536	2.413310
4	6	2.056118	0.038937	2.514939
5	6	0.773608	-2.042459	2.508942
6	6	-0.464737	-2.676667	1.839217
7	7	-1.467105	-1.657263	1.432368
8	6	-1.993068	-0.919250	2.612164
9	6	-2.386983	0.530240	2.333156
10	6	-1.086081	2.533277	1.975424
11	6	0.145455	3.024733	1.215313
12	6	2.282932	2.524158	0.227097

13	6	-2.569661	-2.247988	0.628995
14	8	-0.863275	-2.108016	-1.879141
15	1	0.933569	1.731471	3.154412
16	1	2.591997	2.112882	2.713522
17	1	2.981397	-0.221514	1.993302
18	1	2.182096	-0.208315	3.577050
19	1	0.650763	-1.954869	3.596102
20	1	1.648559	-2.672218	2.311808
21	1	-0.149645	-3.200478	0.934110
22	1	-0.889376	-3.422201	2.529861
23	1	-1.214279	-0.901948	3.374378
24	1	-2.855461	-1.449615	3.044332
25	1	-3.307083	0.620193	1.748068
26	1	-2.553067	1.028394	3.297129
27	1	-0.960605	2.614698	3.064129
28	1	-1.949069	3.150650	1.693686
29	1	-0.148051	3.291359	0.198233
30	1	0.524230	3.931563	1.714018
31	1	1.803099	2.997976	-0.638239
32	1	2.853209	3.309155	0.747789
33	1	-2.130340	-2.959858	-0.076026
34	1	-3.275415	-2.798278	1.268860
35	1	-0.837791	-1.719596	-2.770452
36	1	0.022185	-2.527639	-1.757271
37	8	0.971317	-0.725116	1.973182
38	8	-1.309436	1.164068	1.639102
39	6	3.211763	1.435160	-0.261269
40	6	4.583616	1.620819	-0.441470
41	6	5.351134	0.549686	-0.906487
42	1	5.040484	2.580193	-0.218608
43	6	3.362726	-0.786851	-0.922046
44	6	4.735863	-0.678970	-1.142919
45	1	6.419418	0.670299	-1.060847
46	1	5.280614	-1.554721	-1.476898
47	6	-3.296651	-1.180147	-0.170085
48	6	-4.669564	-1.203567	-0.421245
49	6	-3.064008	0.830048	-1.326127
50	6	-5.235459	-0.163374	-1.165013
51	1	-5.284394	-2.012372	-0.038242
52	6	-4.428110	0.881503	-1.614262
53	1	-6.301106	-0.162943	-1.374732
54	1	-4.818502	1.727296	-2.168570
55	7	-2.525188	-0.187700	-0.638843
56	7	2.619468	0.259101	-0.519143
57	6	2.630729	-2.112584	-1.083240
58	8	1.382229	-2.069213	-0.697150
59	8	3.230030	-3.077088	-1.530680
60	6	-2.104476	1.942426	-1.737788
61	8	-2.545099	2.957749	-2.248468
62	8	-0.840626	1.682898	-1.479147
63	8	0.603717	0.092368	-2.873801
64	1	0.180832	0.979513	-2.881493
65	1	1.461054	0.159204	-3.322345

E(RB3LYP) = -1713.17446784 Hartrees
Corrección de punto cero = 0.530194
Suma de las entalpías electrónicas y térmicas = -1712.609759
Suma de las energías libres y térmicas = -1712.706705

$[Gd(dpa12c4)(H_2O)_2]^+$ (vacío) Λ(δλδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	-0.022064	-0.014116	0.061791
2	7	-1.650263	-1.916468	1.012280
3	6	-0.770464	-2.834707	1.779263
4	6	0.359135	-3.444145	0.950800
5	6	1.751779	-2.946147	-0.933883
6	6	2.444251	-1.815382	-1.700211
7	7	1.635799	-0.590555	-1.950535
8	6	0.768797	-0.653993	-3.153795
9	6	-0.347518	-1.694857	-3.051383
10	6	-1.736766	-2.765951	-1.412299
11	6	-2.444987	-2.559262	-0.069826
12	6	-2.578808	-1.212736	1.948465
13	6	2.550228	0.590235	-2.030335
14	8	0.026260	2.349895	0.882343
15	1	-1.345893	-3.660855	2.227866
16	1	-0.332066	-2.241334	2.585000
17	1	1.088788	-3.537303	-1.576412
18	1	2.529099	-3.625649	-0.558818
19	1	3.313283	-1.509925	-1.116110
20	1	2.825655	-2.228862	-2.647190
21	1	1.354805	-0.874419	-4.060926
22	1	0.317346	0.334020	-3.268019
23	1	-1.063926	-3.631087	-1.399716
24	1	-2.506103	-2.965162	-2.170772
25	1	-3.305820	-1.914855	-0.254640
26	1	-2.838112	-3.533519	0.261682
27	1	-3.340458	-1.898626	2.348431
28	1	-1.978305	-0.856778	2.793707
29	1	3.317735	0.451932	-2.806260
30	1	1.943880	1.457609	-2.317378
31	1	0.227152	3.120156	0.269051
32	1	0.333635	2.563809	1.775617
33	8	0.996214	-2.423895	0.162102
34	8	-0.994026	-1.598616	-1.771172
35	6	-3.232881	-0.024959	1.261944
36	6	-4.525392	0.433018	1.521696
37	6	-4.988045	1.552800	0.822204
38	1	-5.154966	-0.069124	2.249703
39	6	-2.898097	1.643340	-0.338275
40	6	-4.168553	2.173928	-0.122411
41	1	-5.988228	1.931882	1.010698
42	1	-4.486004	3.044125	-0.685371
43	6	3.193071	0.845490	-0.675901
44	6	4.491032	1.317553	-0.482880
45	6	2.833695	0.699693	1.630185
46	6	4.949361	1.485733	0.829172
47	1	5.130631	1.542887	-1.330635
48	6	4.120118	1.164006	1.904672
49	1	5.956488	1.852054	1.006023
50	1	4.437065	1.257057	2.937185
51	7	2.401619	0.564055	0.368237
52	7	-2.458414	0.582761	0.354601
53	6	-1.886206	2.228846	-1.316908
54	8	-0.857336	1.481629	-1.548646
55	8	-2.078266	3.365603	-1.760713

56	6	1.834011	0.311355	2.726735
57	8	2.186805	0.386601	3.893201
58	8	0.667104	-0.066267	2.272913
59	1	-1.079056	-1.512752	-3.848486
60	1	0.038586	-2.713412	-3.181307
61	1	-0.008923	-4.233817	0.284182
62	1	1.093358	-3.897914	1.628115
63	8	0.442714	4.210053	-0.986600
64	1	-0.372016	4.020814	-1.514014
65	1	0.380980	5.150743	-0.757530

E(RB3LYP) = -1713.187381 Hartrees
Corrección de punto cero = 0.530417 Hartrees
Suma de las entalpías electrónicas y térmicas = -1712.622838 Hartrees
Suma de las energías libres y térmicas = -1712.718403 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.056519	-0.148166	-0.081045
2	7	2.707343	-1.489847	-0.296262
3	7	-1.668982	-0.257803	2.172757
4	8	1.147918	-1.110743	2.171941
5	8	-1.788460	-2.265066	0.116956
6	8	0.319880	-2.587063	-1.400511
7	6	-2.496190	-1.488271	2.253279
8	6	-2.959882	-2.015072	0.902491
9	6	-2.052604	-2.772579	-1.199511
10	6	-0.785495	-3.444332	-1.697823
11	6	1.579358	-3.014750	-1.930464
12	1	1.805066	-2.423983	-2.826207
13	1	1.528244	-4.068509	-2.228466
14	6	2.627302	-2.867386	-0.835415
15	1	2.347239	-3.539098	-0.019548
16	1	3.607728	-3.204217	-1.210811
17	6	3.273187	-1.491924	1.076132
18	1	3.572919	-0.469696	1.316878
19	1	4.177570	-2.120810	1.129499
20	6	3.532699	-0.647724	-1.200534
21	1	3.148508	-0.777643	-2.219443
22	1	4.577948	-0.996984	-1.212990
23	6	2.304258	-1.960869	2.158335
24	1	1.985430	-3.003177	2.022105
25	1	2.817763	-1.892171	3.126057
26	6	0.362405	-1.194347	3.373121
27	1	1.002507	-0.978903	4.238653
28	1	-0.015574	-2.219031	3.485973
29	6	-0.748760	-0.147716	3.337721
30	1	-0.284201	0.840133	3.281938
31	1	-1.298113	-0.210303	4.291457
32	6	3.493535	0.824459	-0.841221
33	6	4.586347	1.664731	-1.056779
34	1	5.502237	1.272260	-1.488019
35	6	4.480142	3.012031	-0.702848
36	1	5.313959	3.687239	-0.871249
37	6	3.308654	3.468632	-0.103325
38	1	3.177285	4.491463	0.230318
39	6	2.266593	2.563731	0.095110

40	6	0.995932	2.969488	0.838805
41	7	2.351433	1.278904	-0.299092
42	6	-2.518193	0.966529	2.097727
43	1	-1.866115	1.819777	2.309017
44	1	-3.305464	0.936325	2.865952
45	6	-3.122091	1.223015	0.729674
46	6	-4.354936	1.856297	0.561298
47	1	-4.964155	2.108889	1.423705
48	6	-4.779454	2.171257	-0.732873
49	1	-5.732368	2.669691	-0.885320
50	6	-3.971715	1.845010	-1.821346
51	1	-4.245933	2.069719	-2.845664
52	6	-2.758234	1.204056	-1.574636
53	6	-1.803023	0.817439	-2.706833
54	7	-2.360278	0.899971	-0.327446
55	8	-0.678752	0.290706	-2.288427
56	8	-2.146537	1.004057	-3.861518
57	8	0.891858	4.113321	1.252040
58	8	0.138443	1.997073	0.982305
59	1	-0.633769	-4.409386	-1.195408
60	1	-0.866681	-3.613102	-2.778902
61	1	-2.346819	-1.946596	-1.857004
62	1	-2.864693	-3.509804	-1.168513
63	1	-1.900748	-2.277303	2.718439
64	1	-3.374646	-1.325670	2.896767
65	1	-3.621369	-1.314624	0.382826
66	1	-3.505765	-2.956125	1.055028

E(RB3LYP) = -1709.8299463 Hartrees
Corrección de punto cero = 0.540801 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.255781 Hartrees
Suma de las energías libres y térmicas = -1709.351631 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.060965	-0.146731	-0.060266
2	7	2.656164	-1.582708	-0.298769
3	7	-1.641564	-0.104474	2.186616
4	8	1.137837	-1.073503	2.185032
5	8	-1.971502	-2.031281	0.115540
6	8	0.183080	-2.780412	-1.125146
7	6	-2.503282	-1.302843	2.333403
8	6	-3.063259	-1.839875	1.021636
9	6	-2.145805	-3.107239	-0.814114
10	6	-1.035218	-3.017941	-1.847045
11	6	1.382063	-3.078522	-1.842480
12	1	1.490452	-2.398975	-2.699452
13	1	1.342524	-4.106349	-2.227715
14	6	2.521506	-2.956982	-0.842228
15	1	2.306336	-3.640716	-0.016582
16	1	3.462996	-3.293438	-1.303753
17	6	3.226144	-1.597624	1.072285
18	1	3.581885	-0.589803	1.298897
19	1	4.095668	-2.273147	1.132370
20	6	3.508033	-0.779700	-1.214342
21	1	3.115389	-0.911371	-2.230226
22	1	4.539772	-1.167219	-1.226024

23	6	2.236625	-1.999643	2.164204
24	1	1.847235	-3.017830	2.029109
25	1	2.760273	-1.963488	3.128075
26	6	0.373967	-1.064559	3.403876
27	1	1.039464	-0.829263	4.244626
28	1	-0.039168	-2.066858	3.577014
29	6	-0.700137	0.021689	3.334768
30	1	-0.202535	0.989227	3.229897
31	1	-1.238172	0.019233	4.297027
32	6	3.524376	0.697540	-0.878540
33	6	4.646214	1.493149	-1.115338
34	1	5.545508	1.058865	-1.541639
35	6	4.589993	2.850698	-0.790708
36	1	5.446977	3.491751	-0.976091
37	6	3.436989	3.362255	-0.199844
38	1	3.342178	4.396896	0.109186
39	6	2.364593	2.499292	0.022581
40	6	1.110744	2.968232	0.756313
41	7	2.401801	1.203235	-0.341230
42	6	-2.451804	1.143968	2.061637
43	1	-1.771055	1.983132	2.234801
44	1	-3.237378	1.171408	2.831686
45	6	-3.053590	1.354458	0.683190
46	6	-4.282423	1.988030	0.485303
47	1	-4.886741	2.291956	1.334640
48	6	-4.711029	2.231757	-0.822836
49	1	-5.660440	2.729366	-0.998694
50	6	-3.916909	1.829082	-1.896192
51	1	-4.202862	1.986665	-2.929859
52	6	-2.705901	1.195251	-1.619749
53	6	-1.778622	0.699748	-2.732742
54	7	-2.298973	0.973853	-0.359084
55	8	-0.649077	0.191670	-2.297411
56	8	-2.145656	0.783699	-3.892011
57	8	1.039663	4.129084	1.127009
58	8	0.227495	2.025847	0.939910
59	1	-1.905415	-2.102033	2.777578
60	1	-3.337178	-1.100955	3.024814
61	1	-3.802341	-1.171229	0.568296
62	1	-3.550818	-2.801819	1.226102
63	1	-0.973844	-3.964670	-2.398764
64	1	-1.201156	-2.196546	-2.552940
65	1	-2.099206	-4.058104	-0.266649
66	1	-3.119706	-3.032549	-1.314896

E(RB3LYP) = -1709.8320387 Hartrees
Corrección de punto cero = 0.540866 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.257973 Hartrees
Suma de las energías libres y térmicas = -1709.352934 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.028120	-0.110701	-0.114021
2	7	2.696452	-1.509297	-0.335945
3	7	-1.714354	-0.122936	2.124628
4	8	1.038862	-1.178708	2.107239
5	8	-1.887281	-2.202927	0.140297

6	8	0.296392	-2.641918	-1.279536
7	6	-2.716616	-1.221244	2.170749
8	1	-2.990840	-1.454185	3.211489
9	1	-3.619249	-0.856201	1.675404
10	6	-2.320723	-2.511641	1.466005
11	1	-1.527096	-3.065939	1.985554
12	1	-3.205854	-3.161220	1.430223
13	6	-1.871626	-3.346860	-0.725532
14	1	-2.887598	-3.561349	-1.081042
15	1	-1.496586	-4.216958	-0.170254
16	6	-0.940799	-3.046240	-1.883097
17	1	-0.799211	-3.952083	-2.484844
18	1	-1.313833	-2.240480	-2.524216
19	6	1.500701	-2.939219	-1.986119
20	1	1.635262	-2.239041	-2.821511
21	1	1.456973	-3.955948	-2.397633
22	6	2.614130	-2.855840	-0.952130
23	1	2.391876	-3.587777	-0.171254
24	1	3.575379	-3.145915	-1.404024
25	6	3.196839	-1.573432	1.058785
26	1	3.504369	-0.566380	1.350332
27	1	4.086061	-2.221746	1.133553
28	6	3.570502	-0.654784	-1.177639
29	1	3.226172	-0.755315	-2.214365
30	1	4.609976	-1.021108	-1.158450
31	6	2.172962	-2.062989	2.082924
32	1	1.828753	-3.085830	1.880876
33	1	2.654414	-2.058978	3.069030
34	6	0.245896	-1.231644	3.308097
35	1	0.899193	-1.074829	4.176114
36	1	-0.206976	-2.226013	3.406249
37	6	-0.790939	-0.109266	3.286603
38	1	-0.255370	0.843551	3.255619
39	1	-1.346822	-0.152223	4.238060
40	6	3.543946	0.808160	-0.790512
41	6	4.664422	1.624336	-0.953776
42	1	5.585750	1.212885	-1.354703
43	6	4.578843	2.969570	-0.589637
44	1	5.434319	3.626175	-0.718111
45	6	3.395506	3.446183	-0.031150
46	1	3.273413	4.467812	0.309590
47	6	2.326456	2.563718	0.116843
48	6	1.043369	2.996290	0.817280
49	7	2.390921	1.279927	-0.287259
50	6	-2.444189	1.181817	2.045249
51	1	-1.708590	1.977155	2.192444
52	1	-3.203453	1.252070	2.837932
53	6	-3.074716	1.396662	0.682024
54	6	-4.296608	2.046505	0.501374
55	1	-4.875585	2.374033	1.359376
56	6	-4.751732	2.276807	-0.800600
57	1	-5.697406	2.785803	-0.962709
58	6	-3.987527	1.847438	-1.884405
59	1	-4.292199	1.996493	-2.913872
60	6	-2.780377	1.198756	-1.624876
61	6	-1.875716	0.693770	-2.750326
62	7	-2.351163	0.983966	-0.371211
63	8	-0.736672	0.190254	-2.331096
64	8	-2.258802	0.772860	-3.904284
65	8	0.950908	4.137731	1.239926

66	8	0.158705	2.044051	0.919460

E(RB3LYP) = -1709.828853 Hartrees
Corrección de punto cero = 0.540623 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.254911 Hartrees
Suma de las energías libres y térmicas = -1709.350586 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(δδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.026440	-0.218798	-0.130044
2	7	2.848482	-1.273781	-0.160089
3	7	-1.892953	-0.620640	1.970581
4	8	0.939889	-1.310422	2.101119
5	8	-1.692457	-2.445597	-0.269234
6	8	0.691654	-2.555824	-1.428986
7	6	-2.918373	-1.640421	1.624221
8	1	-3.472719	-1.959466	2.520836
9	1	-3.638201	-1.175908	0.947736
10	6	-2.358005	-2.865372	0.926735
11	1	-1.652276	-3.427792	1.555454
12	1	-3.191378	-3.534254	0.674017
13	6	-1.443680	-3.524284	-1.179609
14	1	-2.377530	-3.819051	-1.676093
15	1	-1.048542	-4.385424	-0.623488
16	6	-0.418433	-3.055901	-2.194056
17	1	-0.106566	-3.900090	-2.819488
18	1	-0.803449	-2.254466	-2.834429
19	6	2.007996	-2.841345	-1.903986
20	1	2.251319	-2.194890	-2.757455
21	1	2.068991	-3.883926	-2.241472
22	6	2.943900	-2.641173	-0.718244
23	1	2.650389	-3.355833	0.054814
24	1	3.977374	-2.885334	-1.013028
25	6	3.261014	-1.220928	1.264879
26	1	3.383017	-0.168779	1.531073
27	1	4.238211	-1.712054	1.416186
28	6	3.674968	-0.355418	-0.983036
29	1	3.424145	-0.533780	-2.035325
30	1	4.746726	-0.591340	-0.875562
31	6	2.266465	-1.852612	2.245003
32	1	2.187501	-2.936073	2.104624
33	1	2.632951	-1.676987	3.262044
34	6	0.310038	-0.656463	3.233000
35	6	-1.177835	-1.003519	3.221020
36	6	3.444214	1.105941	-0.659045
37	6	4.438399	2.068834	-0.841945
38	1	5.410227	1.784935	-1.234489
39	6	4.161599	3.394875	-0.502440
40	1	4.914305	4.164037	-0.648718
41	6	2.927732	3.708932	0.064615
42	1	2.669279	4.707539	0.397728
43	6	1.998164	2.685239	0.237384
44	6	0.688883	2.912052	0.984904
45	7	2.238554	1.422097	-0.162861
46	6	-2.563889	0.706991	2.096531
47	1	-1.820503	1.425958	2.451616
48	1	-3.383779	0.655210	2.829352

49	6	-3.087802	1.200426	0.757997
50	6	-4.246177	1.968904	0.635863
51	1	-4.835846	2.215771	1.513394
52	6	-4.627236	2.417122	-0.632445
53	1	-5.522724	3.020896	-0.747541
54	6	-3.857115	2.079890	-1.744518
55	1	-4.109710	2.393782	-2.750759
56	6	-2.712818	1.308370	-1.544573
57	6	-1.795413	0.906353	-2.701417
58	7	-2.353047	0.886569	-0.321500
59	8	-0.690185	0.305474	-2.319146
60	8	-2.134530	1.154200	-3.844669
61	8	0.405463	4.035085	1.370795
62	8	0.005563	1.815974	1.171149
63	1	-1.265934	-2.086728	3.345523
64	1	-1.652586	-0.540095	4.098568
65	1	0.753532	-1.026356	4.163846
66	1	0.476683	0.422209	3.151404

E(RB3LYP) = -1709.8233795 Hartrees
Corrección de punto cero = 0.540340 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.249661 Hartrees
Suma de las energías libres y térmicas = -1709.345637 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.052357	-0.071826	-0.153494
2	7	2.661917	-1.579706	-0.436893
3	7	-1.557190	-0.204659	2.191699
4	8	1.198274	-1.160944	2.063159
5	8	-1.793102	-2.138656	0.087941
6	8	0.262792	-2.446730	-1.598049
7	6	-2.366119	-1.442362	2.314574
8	6	-2.895511	-1.990278	0.995317
9	6	-1.986685	-3.144220	-0.918565
10	6	-1.027353	-2.852528	-2.069155
11	6	1.066398	-3.448966	-0.976347
12	6	2.504085	-2.943570	-1.011722
13	6	3.274173	-1.606998	0.910480
14	1	3.614119	-0.597124	1.149702
15	1	4.158809	-2.265579	0.932512
16	6	3.461105	-0.732192	-1.365911
17	1	2.980681	-0.795940	-2.349571
18	1	4.484252	-1.123239	-1.482293
19	6	2.327169	-2.047738	2.019881
20	1	1.976708	-3.081036	1.891091
21	1	2.867856	-1.995426	2.973480
22	6	0.505263	-1.156355	3.321543
23	6	-0.582165	-0.086432	3.309799
24	6	3.523588	0.721369	-0.941496
25	6	4.668512	1.496566	-1.126746
26	1	5.556263	1.062007	-1.575870
27	6	4.651558	2.833752	-0.720851
28	1	5.528233	3.458421	-0.864959
29	6	3.512419	3.343466	-0.103116
30	1	3.447913	4.359508	0.268729
31	6	2.412190	2.502149	0.062383

32	6	1.169714	2.967603	0.819923
33	7	2.413307	1.230199	-0.378909
34	6	-2.415024	1.015637	2.168389
35	1	-1.754042	1.871287	2.340255
36	1	-3.152730	0.982586	2.984201
37	6	-3.102061	1.261079	0.839904
38	6	-4.365550	1.846524	0.740616
39	1	-4.936057	2.075959	1.635401
40	6	-4.872544	2.142181	-0.528184
41	1	-5.850499	2.604013	-0.628367
42	6	-4.115786	1.839523	-1.659050
43	1	-4.456808	2.044743	-2.667272
44	6	-2.866298	1.246791	-1.478910
45	6	-1.973041	0.871197	-2.661629
46	7	-2.384907	0.968666	-0.256076
47	8	-0.807013	0.387041	-2.308775
48	8	-2.395850	1.018530	-3.795437
49	8	1.147708	4.097215	1.280939
50	8	0.242241	2.054844	0.922750
51	1	3.157036	-3.665099	-0.500651
52	1	2.816622	-2.919741	-2.059178
53	1	0.997922	-4.391750	-1.535555
54	1	0.717340	-3.635164	0.049076
55	1	-0.937614	-3.732443	-2.719199
56	1	-1.373118	-2.004173	-2.661898
57	1	-1.812356	-4.130578	-0.467634
58	1	-3.016119	-3.117463	-1.297430
59	1	-3.348746	-2.970609	1.190636
60	1	-3.653863	-1.345103	0.540524
61	1	-1.739481	-2.220418	2.755120
62	1	-3.214221	-1.287514	3.000088
63	1	-0.102816	0.890507	3.206278
64	1	-1.087962	-0.112844	4.289139
65	1	1.212593	-0.909986	4.124255
66	1	0.115220	-2.162784	3.522827

E(RB3LYP) = -1709.8261075 Hartrees
Corrección de punto cero = 0.541243 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.251707 Hartrees
Suma de las energías libres y térmicas = -1709.346662 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	-0.010408	0.176735	-0.099994
2	7	-2.501610	1.900500	-0.001558
3	7	1.358583	-0.763869	2.159276
4	8	-1.343488	0.265573	2.201541
5	8	1.964494	1.766462	0.980730
6	8	0.108224	2.965319	-0.373999
7	6	2.071831	0.314038	2.883765
8	6	2.854964	1.258593	1.979545
9	6	2.317191	3.058088	0.465597
10	6	1.439079	3.344502	-0.743243
11	6	-0.945859	3.445484	-1.213889
12	1	-0.972481	2.874212	-2.152835
13	1	-0.779010	4.501771	-1.462396
14	6	-2.216859	3.315347	-0.388903

15	1	-2.072623	3.907786	0.517237
16	1	-3.064522	3.757249	-0.931506
17	6	-3.021346	1.831566	1.391513
18	6	-3.438886	1.335261	-1.004245
19	1	-3.064000	1.630139	-1.992933
20	1	-4.435544	1.793625	-0.898701
21	6	-2.758310	0.541120	2.167973
22	6	-0.864591	-0.435052	3.367773
23	1	-1.665718	-1.057554	3.782603
24	1	-0.592748	0.307918	4.127078
25	6	0.291111	-1.370005	3.003045
26	1	-0.111473	-2.206678	2.428904
27	1	0.704218	-1.769324	3.944279
28	6	-3.571346	-0.171551	-0.993416
29	6	-4.785609	-0.791192	-1.293342
30	1	-5.669785	-0.192376	-1.489357
31	6	-4.839678	-2.185930	-1.340884
32	1	-5.771133	-2.689300	-1.582944
33	6	-3.690917	-2.917646	-1.052879
34	1	-3.667557	-4.001180	-1.044312
35	6	-2.519810	-2.226841	-0.741078
36	6	-1.261762	-2.981166	-0.317669
37	7	-2.458053	-0.880467	-0.736585
38	6	2.286665	-1.844669	1.709735
39	1	1.669779	-2.725445	1.507455
40	1	2.991411	-2.102687	2.514331
41	6	3.036891	-1.551628	0.423031
42	6	4.305281	-2.077094	0.163871
43	1	4.831090	-2.644056	0.926095
44	6	4.874268	-1.872650	-1.095964
45	1	5.856186	-2.278884	-1.320675
46	6	4.174133	-1.146197	-2.058591
47	1	4.565193	-0.956415	-3.051511
48	6	2.918241	-0.643196	-1.721790
49	6	2.089044	0.180552	-2.709726
50	7	2.378387	-0.846859	-0.508322
51	8	0.909459	0.529008	-2.252489
52	8	2.569041	0.467716	-3.792862
53	8	-1.298078	-4.200904	-0.261179
54	8	-0.260346	-2.207823	-0.010921
55	1	1.329941	0.914561	3.416866
56	1	2.755988	-0.106885	3.638508
57	1	3.708909	0.770681	1.496105
58	1	3.235019	2.085178	2.593716
59	1	-3.121352	0.702711	3.190210
60	1	-3.278189	-0.326756	1.751398
61	1	-4.107305	2.021418	1.419246
62	1	-2.540145	2.634718	1.955174
63	1	1.481065	4.416529	-0.975726
64	1	1.751573	2.775203	-1.625036
65	1	2.155329	3.805387	1.253430
66	1	3.373223	3.078213	0.167339

E(RB3LYP) = -1709.8238988 Hartrees
Corrección de punto cero = 0.540883 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.249714 Hartrees
Suma de las energías libres y térmicas = -1709.345333 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(δλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	-0.010125	-0.258299	-0.115692
2	7	2.785717	-1.527884	-0.089976
3	7	-1.811986	-0.333964	2.095582
4	8	1.125076	-0.786571	2.278551
5	8	-1.782939	-2.412422	0.097232
6	8	0.479990	-2.686963	-1.249617
7	6	-2.864114	-1.378023	1.965864
8	1	-3.338628	-1.577275	2.939282
9	1	-3.638572	-0.990811	1.300992
10	6	-2.366531	-2.686152	1.376526
11	1	-1.624922	-3.188988	2.014474
12	1	-3.222457	-3.363347	1.258715
13	6	-1.637251	-3.576705	-0.727405
14	6	-0.701818	-3.221784	-1.867741
15	6	1.751856	-3.027686	-1.804808
16	1	1.974582	-2.381091	-2.663822
17	1	1.742702	-4.066578	-2.157783
18	6	2.756963	-2.897742	-0.668388
19	1	2.448554	-3.595684	0.113715
20	1	3.753843	-3.212606	-1.016102
21	6	3.222659	-1.557382	1.335161
22	6	3.661378	-0.689038	-0.943785
23	1	3.412235	-0.910351	-1.988624
24	1	4.717076	-0.977703	-0.811431
25	6	2.547887	-0.558983	2.276959
26	6	0.411384	-0.036748	3.288620
27	6	-1.026052	-0.543304	3.342571
28	6	3.516143	0.801589	-0.734155
29	6	4.587922	1.670304	-0.951501
30	1	5.556508	1.278520	-1.247167
31	6	4.391016	3.041689	-0.781682
32	1	5.205682	3.737514	-0.959639
33	6	3.148612	3.498504	-0.347346
34	1	2.939149	4.544341	-0.154394
35	6	2.139367	2.564560	-0.120789
36	6	0.813284	2.976713	0.507399
37	7	2.308856	1.247422	-0.353196
38	6	-2.467535	1.007212	2.074339
39	1	-1.703255	1.759773	2.286968
40	1	-3.244854	1.066231	2.851519
41	6	-3.057962	1.323975	0.710852
42	6	-4.214122	2.087192	0.544496
43	1	-4.762307	2.449078	1.408897
44	6	-4.644961	2.383457	-0.752214
45	1	-5.539699	2.980333	-0.903131
46	6	-3.922273	1.908202	-1.845337
47	1	-4.210584	2.106443	-2.871219
48	6	-2.777504	1.150684	-1.599829
49	6	-1.903731	0.612808	-2.733788
50	7	-2.374473	0.867891	-0.350790
51	8	-0.785770	0.056183	-2.322622
52	8	-2.283635	0.724304	-3.885604
53	8	0.590193	4.159121	0.713596
54	8	0.050345	1.963666	0.811037
55	1	-0.989593	-1.618815	3.541037

56	1	-1.529625	-0.074662	4.202021
57	1	0.882093	-0.213779	4.264126
58	1	0.466496	1.031265	3.050382
59	1	2.937941	-0.738368	3.287913
60	1	2.750526	0.481719	2.008514
61	1	4.310823	-1.408630	1.415777
62	1	3.009992	-2.555303	1.727851
63	1	-0.462394	-4.122365	-2.444345
64	1	-1.129298	-2.465668	-2.535026
65	1	-1.207736	-4.393495	-0.131718
66	1	-2.617754	-3.889513	-1.109358

E(RB3LYP) = -1709.8240453 Hartrees
Corrección de punto cero = 0.540831 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.250054 Hartrees
Suma de las energías libres y térmicas = -1709.345213 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	0.007297	-0.064206	-0.164273
2	7	2.701314	-1.458520	-0.358218
3	7	-1.681550	-0.219028	2.131837
4	8	1.062976	-1.200646	2.071822
5	8	-1.837393	-2.133258	0.036748
6	8	0.310367	-2.553084	-1.590443
7	6	-2.561593	-1.416055	2.188395
8	1	-2.726355	-1.734861	3.228989
9	1	-3.534493	-1.132260	1.779491
10	6	-2.069032	-2.604105	1.367241
11	1	-1.155670	-3.056128	1.774215
12	1	-2.850791	-3.374532	1.360044
13	6	-1.914287	-3.093034	-1.026394
14	6	-0.545383	-3.666966	-1.336913
15	6	1.611857	-2.871547	-2.094528
16	1	1.821870	-2.147532	-2.887611
17	1	1.612987	-3.868606	-2.549849
18	6	2.634511	-2.807840	-0.966407
19	1	2.337730	-3.523565	-0.194031
20	1	3.623746	-3.127939	-1.333729
21	6	3.226442	-1.520989	1.026384
22	1	3.514779	-0.509591	1.321152
23	1	4.131811	-2.149121	1.079738
24	6	3.558979	-0.583829	-1.198008
25	1	3.212068	-0.670489	-2.234287
26	1	4.603061	-0.937274	-1.188896
27	6	2.229204	-2.038092	2.058924
28	1	1.927456	-3.078361	1.875351
29	1	2.714185	-2.003099	3.042633
30	6	0.323370	-1.221304	3.305953
31	1	1.005910	-1.010652	4.139225
32	1	-0.099223	-2.221947	3.466542
33	6	-0.742600	-0.132027	3.276017
34	1	-0.241762	0.836887	3.203113
35	1	-1.281451	-0.165598	4.237834
36	6	3.516202	0.873748	-0.785894
37	6	4.626525	1.705977	-0.934607
38	1	5.551740	1.314391	-1.346350

39	6	4.526145	3.042110	-0.540660
40	1	5.373666	3.711056	-0.657697
41	6	3.340249	3.493156	0.033489
42	1	3.209202	4.505327	0.398250
43	6	2.281033	2.596017	0.165166
44	6	0.996438	2.997736	0.884528
45	7	2.359658	1.323381	-0.270080
46	6	-2.517516	1.019440	2.085145
47	1	-1.845319	1.866396	2.251074
48	1	-3.270623	1.010923	2.886631
49	6	-3.176135	1.229378	0.735562
50	6	-4.456604	1.765224	0.590673
51	1	-5.061961	1.983700	1.465073
52	6	-4.935499	2.029010	-0.696579
53	1	-5.927106	2.451348	-0.830953
54	6	-4.132741	1.748654	-1.800590
55	1	-4.448982	1.935728	-2.820347
56	6	-2.867468	1.205246	-1.576751
57	6	-1.915483	0.872703	-2.728196
58	7	-2.418065	0.952021	-0.337538
59	8	-0.740511	0.442127	-2.331977
60	8	-2.297998	1.013946	-3.876113
61	8	0.899130	4.126327	1.338593
62	8	0.118840	2.036026	0.968812
63	1	-0.161208	-4.270977	-0.500778
64	1	-0.610060	-4.308646	-2.225619
65	1	-2.289619	-2.547720	-1.896286
66	1	-2.623968	-3.889271	-0.772591

E(RB3LYP) = -1709.8239253 Hartrees
Corrección de punto cero = 0.540615 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.249955 Hartrees
Suma de las energías libres y térmicas = -1709.345892 Hartrees

[La(dpa15c5)]$^{+}$ (vacío) Λ(λλ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	-0.038913	0.127121	-0.203677
2	7	-2.685401	1.503563	-0.525926
3	7	1.543533	-0.100114	2.181467
4	8	-1.248213	0.876833	2.040226
5	8	1.852154	2.083580	0.435569
6	8	-0.259556	3.001893	-0.865225
7	6	2.420758	1.055736	2.489549
8	6	2.977012	1.740347	1.249222
9	6	2.109529	2.973865	-0.660866
10	6	0.885604	3.854145	-0.789479
11	6	-1.482476	3.725870	-0.771149
12	6	-2.615148	2.818214	-1.211072
13	6	-3.250366	1.587981	0.849085
14	1	-3.711829	0.623504	1.074466
15	1	-4.049616	2.346149	0.892430
16	6	-3.547646	0.629029	-1.372177
17	1	-3.157165	0.684407	-2.395305
18	1	-4.580269	1.011110	-1.407402
19	6	-2.269829	1.885203	1.986962
20	1	-1.796589	2.870561	1.903448
21	1	-2.842700	1.868160	2.923529

22	6	-0.548099	0.797916	3.296818
23	1	-1.263481	0.540220	4.088369
24	1	-0.128122	1.784211	3.533120
25	6	0.517078	-0.298037	3.238826
26	1	0.023511	-1.250743	3.031412
27	1	0.973749	-0.367984	4.239892
28	6	-3.553125	-0.818007	-0.939827
29	6	-4.694761	-1.612467	-1.054991
30	1	-5.619762	-1.187027	-1.431952
31	6	-4.623309	-2.955745	-0.679470
32	1	-5.495463	-3.596546	-0.769860
33	6	-3.428178	-3.450556	-0.165017
34	1	-3.310671	-4.472574	0.176216
35	6	-2.337425	-2.587123	-0.065210
36	6	-1.034885	-3.043225	0.576328
37	7	-2.392069	-1.304357	-0.470346
38	6	2.347597	-1.342990	1.997156
39	1	1.653070	-2.186634	2.034636
40	1	3.078066	-1.454641	2.812460
41	6	3.046130	-1.419115	0.651098
42	6	4.280635	-2.049130	0.481023
43	1	4.813750	-2.449681	1.337801
44	6	4.809297	-2.162612	-0.807983
45	1	5.765608	-2.654306	-0.961064
46	6	4.103571	-1.639952	-1.890799
47	1	4.464394	-1.697513	-2.911270
48	6	2.880660	-1.017718	-1.642445
49	6	2.038388	-0.416418	-2.770558
50	7	2.378923	-0.915614	-0.400221
51	8	0.888065	0.073001	-2.367546
52	8	2.476493	-0.421596	-3.906982
53	8	-0.952650	-4.176233	1.024810
54	8	-0.117356	-2.118777	0.609763
55	1	0.798903	4.506036	0.091522
56	1	0.952556	4.480313	-1.689300
57	1	2.284176	2.394254	-1.574340
58	1	2.989737	3.593998	-0.455625
59	1	-3.567321	3.365779	-1.111383
60	1	-2.466391	2.617512	-2.275763
61	1	-1.610496	4.114723	0.248617
62	1	-1.462365	4.591069	-1.448469
63	1	3.506771	2.653427	1.552049
64	1	3.672463	1.106580	0.691072
65	1	3.252337	0.753250	3.144406
66	1	1.838719	1.801264	3.035980

E(RB3LYP) = -1709.8236577 Hartrees
Corrección de punto cero = 0.541155 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.249274 Hartrees
Suma de las energías libres y térmicas = -1709.344626 Hartrees

[La(dpa15c5)]$^+$ (vacío) Λ(λδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	57	-0.038913	0.127121	-0.203677
2	7	-2.685401	1.503563	-0.525926
3	7	1.543533	-0.100114	2.181467
4	8	-1.248213	0.876833	2.040226

5	8	1.852154	2.083580	0.435569
6	8	-0.259556	3.001893	-0.865225
7	6	2.420758	1.055736	2.489549
8	6	2.977012	1.740347	1.249222
9	6	2.109529	2.973865	-0.660866
10	6	0.885604	3.854145	-0.789479
11	6	-1.482476	3.725870	-0.771149
12	6	-2.615148	2.818214	-1.211072
13	6	-3.250366	1.587981	0.849085
14	1	-3.711829	0.623504	1.074466
15	1	-4.049616	2.346149	0.892430
16	6	-3.547646	0.629029	-1.372177
17	1	-3.157165	0.684407	-2.395305
18	1	-4.580269	1.011110	-1.407402
19	6	-2.269829	1.885203	1.986962
20	1	-1.796589	2.870561	1.903448
21	1	-2.842700	1.868160	2.923529
22	6	-0.548099	0.797916	3.296818
23	1	-1.263481	0.540220	4.088369
24	1	-0.128122	1.784211	3.533120
25	6	0.517078	-0.298037	3.238826
26	1	0.023511	-1.250743	3.031412
27	1	0.973749	-0.367984	4.239892
28	6	-3.553125	-0.818007	-0.939827
29	6	-4.694761	-1.612467	-1.054991
30	1	-5.619762	-1.187027	-1.431952
31	6	-4.623309	-2.955745	-0.679470
32	1	-5.495463	-3.596546	-0.769860
33	6	-3.428178	-3.450556	-0.165017
34	1	-3.310671	-4.472574	0.176216
35	6	-2.337425	-2.587123	-0.065210
36	6	-1.034885	-3.043225	0.576328
37	7	-2.392069	-1.304357	-0.470346
38	6	2.347597	-1.342990	1.997156
39	1	1.653070	-2.186634	2.034636
40	1	3.078066	-1.454641	2.812460
41	6	3.046130	-1.419115	0.651098
42	6	4.280635	-2.049130	0.481023
43	1	4.813750	-2.449681	1.337801
44	6	4.809297	-2.162612	-0.807983
45	1	5.765608	-2.654306	-0.961064
46	6	4.103571	-1.639952	-1.890799
47	1	4.464394	-1.697513	-2.911270
48	6	2.880660	-1.017718	-1.642445
49	6	2.038388	-0.416418	-2.770558
50	7	2.378923	-0.915614	-0.400221
51	8	0.888065	0.073001	-2.367546
52	8	2.476493	-0.421596	-3.906982
53	8	-0.952650	-4.176233	1.024810
54	8	-0.117356	-2.118777	0.609763
55	1	0.798903	4.506036	0.091522
56	1	0.952556	4.480313	-1.689300
57	1	2.284176	2.394254	-1.574340
58	1	2.989737	3.593998	-0.455625
59	1	-3.567321	3.365779	-1.111383
60	1	-2.466391	2.617512	-2.275763
61	1	-1.610496	4.114723	0.248617
62	1	-1.462365	4.591069	-1.448469
63	1	3.506771	2.653427	1.552049
64	1	3.672463	1.106580	0.691072

65	1	3.252337	0.753250	3.144406
66	1	1.838719	1.801264	3.035980

E(RB3LYP) = -1709.8248594 Hartrees
Corrección de punto cero = 0.541179 Hartrees
Suma de las entalpías electrónicas y térmicas = -1709.250454 Hartrees
Suma de las energías libres y térmicas = -1709.346033 Hartrees

[Nd(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	60	0.060111	-0.169995	-0.027798
2	7	2.667321	-1.476376	-0.310044
3	7	-1.694768	-0.323327	2.143676
4	8	1.104735	-1.175160	2.150815
5	8	-1.822181	-2.218419	0.012168
6	8	0.296244	-2.539853	-1.428901
7	6	-2.520070	-1.555564	2.181403
8	6	-2.991993	-2.012787	0.809998
9	6	-2.086637	-2.644089	-1.331972
10	6	-0.827280	-3.313624	-1.854947
11	6	1.547602	-2.957145	-1.980842
12	1	1.771957	-2.346036	-2.863566
13	1	1.490877	-4.004500	-2.301326
14	6	2.595787	-2.839604	-0.884590
15	1	2.318126	-3.534951	-0.088081
16	1	3.577884	-3.160400	-1.268888
17	6	3.238750	-1.509955	1.059334
18	1	3.533386	-0.492550	1.325182
19	1	4.146155	-2.135594	1.094788
20	6	3.483979	-0.609691	-1.198494
21	1	3.098876	-0.722312	-2.218676
22	1	4.532615	-0.948107	-1.217562
23	6	2.272170	-2.011261	2.128855
24	1	1.966144	-3.054256	1.972176
25	1	2.778765	-1.952914	3.100647
26	6	0.316610	-1.282170	3.349911
27	1	0.955063	-1.079446	4.219447
28	1	-0.056838	-2.310293	3.443058
29	6	-0.797907	-0.238809	3.328183
30	1	-0.337186	0.751468	3.304870
31	1	-1.362967	-0.331414	4.270114
32	6	3.425470	0.852393	-0.809499
33	6	4.493879	1.722131	-1.031747
34	1	5.407732	1.359878	-1.492703
35	6	4.365741	3.058454	-0.646027
36	1	5.179939	3.756190	-0.818433
37	6	3.197999	3.475164	-0.010257
38	1	3.051190	4.487528	0.348084
39	6	2.182975	2.541690	0.190694
40	6	0.918150	2.890126	0.965608
41	7	2.287380	1.267793	-0.231726
42	6	-2.549462	0.897081	2.074310
43	1	-1.918797	1.745379	2.355484
44	1	-3.377655	0.829320	2.795396
45	6	-3.077907	1.206941	0.686099
46	6	-4.287784	1.872169	0.476325
47	1	-4.934394	2.110772	1.315178

48	6	-4.640272	2.236861	-0.826075
49	1	-5.574403	2.759891	-1.009173
50	6	-3.784149	1.930266	-1.883269
51	1	-4.000865	2.195311	-2.911724
52	6	-2.597786	1.257360	-1.596413
53	6	-1.585202	0.893231	-2.683475
54	7	-2.271329	0.901130	-0.342113
55	8	-0.489944	0.346458	-2.214235
56	8	-1.859077	1.111165	-3.850921
57	8	0.779243	4.017859	1.410984
58	8	0.097290	1.883907	1.097772
59	1	-0.730080	-4.330560	-1.451022
60	1	-0.870912	-3.367236	-2.949945
61	1	-2.359133	-1.776051	-1.942188
62	1	-2.915082	-3.363104	-1.348992
63	1	-1.919072	-2.364913	2.602606
64	1	-3.392014	-1.422404	2.840425
65	1	-3.655336	-1.285455	0.330505
66	1	-3.537297	-2.960737	0.913481

E(RB3LYP) = -1711.7413125 Hartrees
Corrección de punto cero = 0.541350 Hartrees
Suma de las entalpías electrónicas y térmicas = -1711.166800 Hartrees
Suma de las energías libres y térmicas = -1711.261777 Hartrees

$[Nd(dpa15c5)]^+$ (vacío) Λ(λδ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	60	0.058365	-0.161072	-0.017340
2	7	2.619518	-1.567996	-0.302248
3	7	-1.664661	-0.143350	2.164264
4	8	1.091901	-1.114735	2.168251
5	8	-1.982320	-2.007510	0.054285
6	8	0.166303	-2.736375	-1.173260
7	6	-2.522603	-1.346054	2.285090
8	6	-3.079100	-1.842556	0.958221
9	6	-2.165939	-3.047776	-0.912652
10	6	-1.037813	-2.945963	-1.923328
11	6	1.369546	-3.032850	-1.882343
12	1	1.491315	-2.340185	-2.726237
13	1	1.326172	-4.054425	-2.283480
14	6	2.495711	-2.933834	-0.867135
15	1	2.269610	-3.630624	-0.055637
16	1	3.443813	-3.261368	-1.321328
17	6	3.193156	-1.601129	1.066314
18	1	3.542445	-0.595051	1.309124
19	1	4.066312	-2.272647	1.115093
20	6	3.463425	-0.747625	-1.208694
21	1	3.070627	-0.868937	-2.225187
22	1	4.498969	-1.124332	-1.224566
23	6	2.203776	-2.026080	2.148883
24	1	1.828686	-3.047844	2.003834
25	1	2.719317	-1.989418	3.116786
26	6	0.332603	-1.110819	3.391197
27	1	1.001848	-0.877720	4.229243
28	1	-0.077492	-2.114590	3.561328
29	6	-0.743588	-0.026924	3.328318
30	1	-0.249827	0.943741	3.243438

31	1	-1.294929	-0.048347	4.282611
32	6	3.460256	0.723280	-0.853557
33	6	4.561122	1.545196	-1.099479
34	1	5.459619	1.135421	-1.550743
35	6	4.485102	2.895483	-0.751232
36	1	5.325221	3.556543	-0.942716
37	6	3.334005	3.373718	-0.128827
38	1	3.225114	4.400685	0.200299
39	6	2.284488	2.485420	0.097740
40	6	1.034013	2.906448	0.858168
41	7	2.339053	1.196317	-0.286898
42	6	-2.483236	1.098695	2.036171
43	1	-1.824098	1.940539	2.265595
44	1	-3.306490	1.094908	2.765918
45	6	-3.017015	1.342337	0.635699
46	6	-4.224227	2.001663	0.392568
47	1	-4.862851	2.299298	1.218627
48	6	-4.586059	2.280277	-0.928354
49	1	-5.517483	2.798249	-1.137686
50	6	-3.747583	1.888069	-1.971712
51	1	-3.979602	2.075190	-3.013848
52	6	-2.563036	1.227069	-1.651028
53	6	-1.584430	0.744539	-2.722290
54	7	-2.221919	0.968559	-0.377901
55	8	-0.486318	0.211929	-2.234786
56	8	-1.881943	0.857008	-3.898461
57	8	0.939345	4.050866	1.271574
58	8	0.172889	1.938505	1.016198
59	1	-1.922352	-2.156009	2.705808
60	1	-3.355732	-1.163491	2.982553
61	1	-3.815269	-1.158958	0.522131
62	1	-3.569429	-2.809422	1.129830
63	1	-0.974887	-3.880916	-2.494671
64	1	-1.181036	-2.108509	-2.614219
65	1	-2.146272	-4.016682	-0.396152
66	1	-3.131468	-2.936485	-1.422705

E(RB3LYP) = -1711.7437715 Hartrees
Corrección de punto cero = 0.541375 Hartrees
Suma de las entalpías electrónicas y térmicas = -1711.169326 Hartrees
Suma de las energías libres y térmicas = -1711.263865 Hartrees

[Gd(dpa15c5)]$^{+}$ (vacío) **Λ(λδ)(δλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.060416	-0.183494	0.019497
2	7	2.624915	-1.463876	-0.319193
3	7	-1.732291	-0.395851	2.099949
4	8	1.047560	-1.243193	2.121443
5	8	-1.855990	-2.151749	-0.117049
6	8	0.277132	-2.498728	-1.464841
7	6	-2.558450	-1.626519	2.079585
8	6	-3.029057	-2.001927	0.684721
9	6	-2.107860	-2.508145	-1.482116
10	6	-0.851981	-3.181856	-2.010440
11	6	1.524716	-2.904086	-2.028431
12	1	1.752633	-2.273939	-2.897111
13	1	1.466021	-3.944944	-2.371024

14	6	2.566521	-2.813101	-0.926090
15	1	2.287361	-3.529795	-0.149452
16	1	3.552817	-3.117811	-1.312041
17	6	3.196959	-1.527321	1.048175
18	1	3.483889	-0.515291	1.340903
19	1	4.108018	-2.148127	1.069979
20	6	3.434535	-0.573050	-1.189326
21	1	3.049118	-0.666135	-2.210839
22	1	4.486183	-0.901445	-1.213991
23	6	2.227986	-2.062522	2.097835
24	1	1.937939	-3.106188	1.918772
25	1	2.721223	-2.014046	3.076755
26	6	0.250207	-1.387525	3.312178
27	1	0.882312	-1.206302	4.190736
28	1	-0.117186	-2.420151	3.371960
29	6	-0.869364	-0.350258	3.310253
30	1	-0.415199	0.642098	3.336720
31	1	-1.456914	-0.486639	4.232805
32	6	3.357724	0.877184	-0.768051
33	6	4.400563	1.776829	-0.994222
34	1	5.310643	1.446810	-1.485823
35	6	4.251438	3.099854	-0.573138
36	1	5.045019	3.820460	-0.747466
37	6	3.089346	3.473966	0.099479
38	1	2.927515	4.474159	0.484621
39	6	2.102869	2.511515	0.300204
40	6	0.845242	2.799610	1.104180
41	7	2.226023	1.250644	-0.153638
42	6	-2.588509	0.823370	2.039509
43	1	-1.983042	1.659945	2.398251
44	1	-3.458714	0.717865	2.704267
45	6	-3.032711	1.196056	0.637330
46	6	-4.216335	1.894464	0.386801
47	1	-4.902507	2.117270	1.198132
48	6	-4.491035	2.312085	-0.918054
49	1	-5.403959	2.860439	-1.131476
50	6	-3.584204	2.026640	-1.938788
51	1	-3.739771	2.333458	-2.966712
52	6	-2.427929	1.321554	-1.612374
53	6	-1.356466	0.979590	-2.646939
54	7	-2.178052	0.911059	-0.356768
55	8	-0.294243	0.414186	-2.124511
56	8	-1.555798	1.227576	-3.822983
57	8	0.666818	3.909720	1.577885
58	8	0.067159	1.757418	1.226912
59	1	-0.811351	-4.234105	-1.697367
60	1	-0.843728	-3.136331	-3.106703
61	1	-2.352266	-1.607773	-2.056040
62	1	-2.952478	-3.205111	-1.545727
63	1	-1.956391	-2.457578	2.454768
64	1	-3.428659	-1.526809	2.746889
65	1	-3.694466	-1.248221	0.250155
66	1	-3.571186	-2.956301	0.727268

E(RB3LYP) = -1714.1526672 Hartrees
Corrección de punto cero = 0.541662 Hartrees
Suma de las entalpías electrónicas y térmicas = -1713.577896 Hartrees
Suma de las energías libres y térmicas = -1713.672776 Hartrees

[Gd(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.057172	-0.171541	0.033796
2	7	2.574971	-1.557201	-0.305684
3	7	-1.707883	-0.213785	2.125731
4	8	1.026150	-1.183715	2.144982
5	8	-2.006510	-1.966345	-0.061477
6	8	0.144850	-2.677759	-1.258604
7	6	-2.566071	-1.419469	2.189547
8	6	-3.112527	-1.845505	0.836120
9	6	-2.196050	-2.945141	-1.088662
10	6	-1.034382	-2.827122	-2.057082
11	6	1.358730	-2.968783	-1.948628
12	1	1.505580	-2.254672	-2.769973
13	1	1.313501	-3.979166	-2.377523
14	6	2.460168	-2.907968	-0.905945
15	1	2.209706	-3.623849	-0.118574
16	1	3.418086	-3.228437	-1.344290
17	6	3.145546	-1.625022	1.062070
18	1	3.490095	-0.624817	1.333873
19	1	4.020324	-2.295259	1.096741
20	6	3.420946	-0.715124	-1.189173
21	1	3.038232	-0.818580	-2.210780
22	1	4.459571	-1.083350	-1.200909
23	6	2.149757	-2.082098	2.124077
24	1	1.787831	-3.104815	1.956402
25	1	2.650750	-2.056033	3.099647
26	6	0.257633	-1.211683	3.363732
27	1	0.921648	-0.997142	4.210509
28	1	-0.148676	-2.221265	3.504947
29	6	-0.821773	-0.131289	3.318330
30	1	-0.332394	0.843698	3.280090
31	1	-1.397750	-0.193053	4.256031
32	6	3.398300	0.746572	-0.805966
33	6	4.478010	1.595925	-1.054152
34	1	5.375988	1.213392	-1.529714
35	6	4.381348	2.936636	-0.676938
36	1	5.204357	3.618595	-0.869316
37	6	3.231660	3.378342	-0.024668
38	1	3.107706	4.396137	0.326957
39	6	2.206469	2.463133	0.201233
40	6	0.959583	2.829914	0.988249
41	7	2.279195	1.183441	-0.209943
42	6	-2.529664	1.026667	2.007032
43	1	-1.898033	1.862376	2.318745
44	1	-3.397839	0.980411	2.680868
45	6	-2.975195	1.331852	0.588169
46	6	-4.153192	2.025550	0.299843
47	1	-4.832358	2.308076	1.098451
48	6	-4.433308	2.357625	-1.028229
49	1	-5.341092	2.902159	-1.271195
50	6	-3.543244	1.985306	-2.035958
51	1	-3.710850	2.214403	-3.082079
52	6	-2.392158	1.290386	-1.671145
53	6	-1.355402	0.826491	-2.691801
54	7	-2.130735	0.977575	-0.391162
55	8	-0.295471	0.270824	-2.147479

56	8	-1.574616	0.968310	-3.881750
57	8	0.825825	3.961209	1.425508
58	8	0.138495	1.825909	1.140893
59	1	-1.967556	-2.249371	2.572530
60	1	-3.401847	-1.269057	2.891404
61	1	-3.843322	-1.137915	0.428869
62	1	-3.607513	-2.818354	0.951728
63	1	-0.972870	-3.739142	-2.664792
64	1	-1.134455	-1.960725	-2.718582
65	1	-2.222673	-3.940562	-0.625480
66	1	-3.142878	-2.773911	-1.617058

E(RB3LYP) = -1714.1554533 Hartrees
Corrección de punto cero = 0.541864 Hartrees
Suma de las entalpías electrónicas y térmicas = -1713.580631 Hartrees
Suma de las energías libres y térmicas = -1713.674900 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	0.060718	-0.181386	0.049603
2	7	2.572939	-1.486520	-0.316703
3	7	-1.756034	-0.383426	2.079264
4	8	0.998468	-1.260576	2.109946
5	8	-1.902592	-2.092207	-0.153159
6	8	0.224931	-2.496085	-1.459613
7	6	-2.597033	-1.603061	2.049043
8	6	-3.073897	-1.951598	0.650357
9	6	-2.156483	-2.428707	-1.521882
10	6	-0.912190	-3.125349	-2.048933
11	6	1.464564	-2.914805	-2.026799
12	1	1.699415	-2.287330	-2.895724
13	1	1.394079	-3.955567	-2.368583
14	6	2.505686	-2.834852	-0.924559
15	1	2.219995	-3.550235	-0.149180
16	1	3.490563	-3.145516	-1.309086
17	6	3.151288	-1.558042	1.047287
18	1	3.450679	-0.550285	1.341787
19	1	4.054975	-2.189445	1.065246
20	6	3.383433	-0.601637	-1.191969
21	1	2.983166	-0.683998	-2.208423
22	1	4.431008	-0.941371	-1.229477
23	6	2.176647	-2.085247	2.095055
24	1	1.881900	-3.127825	1.918645
25	1	2.664135	-2.034584	3.076541
26	6	0.199908	-1.398008	3.302253
27	1	0.835472	-1.224569	4.179628
28	1	-0.176515	-2.427408	3.359454
29	6	-0.910573	-0.351475	3.301197
30	1	-0.450598	0.637205	3.342070
31	1	-1.509929	-0.493888	4.215135
32	6	3.323990	0.845268	-0.761490
33	6	4.366089	1.743159	-0.997886
34	1	5.266502	1.414025	-1.507505
35	6	4.228749	3.063176	-0.563706
36	1	5.022066	3.782272	-0.745210
37	6	3.078619	3.436302	0.130082
38	1	2.926320	4.434267	0.524859

39	6	2.092739	2.475377	0.337821
40	6	0.844473	2.753491	1.155548
41	7	2.204549	1.217432	-0.125821
42	6	-2.598229	0.844587	2.003120
43	1	-1.998853	1.672499	2.390269
44	1	-3.491900	0.741372	2.636235
45	6	-2.990423	1.231175	0.589226
46	6	-4.153724	1.949019	0.301164
47	1	-4.862299	2.181838	1.090159
48	6	-4.379857	2.372309	-1.011058
49	1	-5.276642	2.935485	-1.252398
50	6	-3.445755	2.073176	-2.002993
51	1	-3.563620	2.382988	-3.035042
52	6	-2.312075	1.350038	-1.640183
53	6	-1.211625	0.989003	-2.635654
54	7	-2.108928	0.934354	-0.377559
55	8	-0.179052	0.406903	-2.072196
56	8	-1.361622	1.238284	-3.818477
57	8	0.665187	3.855049	1.647897
58	8	0.069612	1.706761	1.266778
59	1	-0.909998	-4.187853	-1.769266
60	1	-0.879691	-3.046405	-3.142935
61	1	-2.380139	-1.517829	-2.087676
62	1	-3.016467	-3.105553	-1.596023
63	1	-2.003125	-2.445963	2.410734
64	1	-3.463256	-1.500881	2.721209
65	1	-3.736930	-1.186772	0.230912
66	1	-3.621519	-2.903489	0.676312

E(RB3LYP) = -1715.9147166 Hartrees
Corrección de punto cero = 0.541939 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.339728 Hartrees
Suma de las energías libres y térmicas = -1715.434522 Hartrees

$[Ho(dpa15c5)]^{+}$ (vacío) Λ(λδ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	0.056686	-0.166384	0.064636
2	7	2.527231	-1.574500	-0.294208
3	7	-1.735100	-0.202408	2.102343
4	8	0.973146	-1.196848	2.138042
5	8	-2.042294	-1.924824	-0.096224
6	8	0.101719	-2.673477	-1.266066
7	6	-2.607707	-1.397686	2.154029
8	6	-3.152279	-1.800823	0.794107
9	6	-2.243281	-2.888061	-1.134931
10	6	-1.065127	-2.791371	-2.084319
11	6	1.316726	-2.975601	-1.946055
12	1	1.477551	-2.262243	-2.765117
13	1	1.265974	-3.985589	-2.375982
14	6	2.407995	-2.925186	-0.893719
15	1	2.143164	-3.638163	-0.108445
16	1	3.368263	-3.253041	-1.321217
17	6	3.098616	-1.647626	1.072428
18	1	3.450520	-0.650807	1.346750
19	1	3.967780	-2.325012	1.107129
20	6	3.377955	-0.739474	-1.179406
21	1	2.990377	-0.837167	-2.199386

22	1	4.413517	-1.116005	-1.193596
23	6	2.095324	-2.098800	2.128655
24	1	1.730759	-3.120407	1.961591
25	1	2.587523	-2.070260	3.108400
26	6	0.201962	-1.219377	3.356607
27	1	0.867469	-1.011156	4.203550
28	1	-0.211222	-2.226434	3.494724
29	6	-0.869459	-0.131991	3.309643
30	1	-0.374969	0.840257	3.287486
31	1	-1.459890	-0.201150	4.237724
32	6	3.365238	0.720174	-0.793346
33	6	4.442052	1.569803	-1.053651
34	1	5.332681	1.188162	-1.543502
35	6	4.351989	2.908986	-0.670060
36	1	5.172844	3.590973	-0.871233
37	6	3.211394	3.349366	-0.000610
38	1	3.093010	4.366180	0.355789
39	6	2.189606	2.433598	0.235006
40	6	0.950403	2.790560	1.033965
41	7	2.255696	1.155144	-0.180103
42	6	-2.543462	1.044954	1.967284
43	1	-1.919547	1.874072	2.309623
44	1	-3.436252	0.998380	2.608007
45	6	-2.934631	1.362904	0.535464
46	6	-4.090036	2.077213	0.207939
47	1	-4.790486	2.371443	0.983604
48	6	-4.320433	2.413614	-1.128471
49	1	-5.210216	2.973551	-1.401138
50	6	-3.404295	2.025304	-2.106627
51	1	-3.533965	2.256210	-3.157743
52	6	-2.277963	1.312271	-1.703378
53	6	-1.213397	0.827154	-2.682602
54	7	-2.064407	0.995128	-0.415569
55	8	-0.182368	0.261827	-2.093661
56	8	-1.385265	0.960868	-3.881085
57	8	0.810693	3.916132	1.482923
58	8	0.136595	1.778885	1.182673
59	1	-2.020285	-2.238545	2.530433
60	1	-3.443504	-1.243175	2.854943
61	1	-3.871834	-1.078904	0.391086
62	1	-3.661288	-2.768131	0.894942
63	1	-1.014948	-3.701947	-2.695742
64	1	-1.135723	-1.921902	-2.745547
65	1	-2.301512	-3.886851	-0.681731
66	1	-3.178665	-2.688085	-1.673768

E(RB3LYP) = -1715.9176441 Hartrees
Corrección de punto cero = 0.542234 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.342531 Hartrees
Suma de las energías libres y térmicas = -1715.436618 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.032467	-0.129311	-0.017135
2	7	-2.556319	-1.544661	0.319857
3	7	1.845855	-0.181368	-2.030966
4	8	-0.830540	-1.324458	-2.046008

5	8	2.009397	-2.060671	0.070125
6	8	-0.176388	-2.542244	1.384664
7	6	2.890807	-1.238781	-1.984644
8	1	3.202310	-1.526378	-3.000326
9	1	3.766431	-0.812379	-1.489376
10	6	2.507418	-2.479784	-1.198868
11	1	1.751530	-3.100239	-1.699853
12	1	3.406932	-3.096236	-1.068729
13	6	2.062287	-3.101241	1.054597
14	1	3.071939	-3.165324	1.480154
15	1	1.812242	-4.060167	0.582104
16	6	1.030377	-2.781285	2.112746
17	1	0.914069	-3.641349	2.784072
18	1	1.287769	-1.899724	2.708573
19	6	-1.387063	-2.822273	2.081417
20	1	-1.565055	-2.061840	2.852451
21	1	-1.323492	-3.803264	2.571247
22	6	-2.462152	-2.852118	1.010952
23	1	-2.183645	-3.619799	0.284646
24	1	-3.432354	-3.145718	1.440076
25	6	-3.027526	-1.698481	-1.076126
26	1	-3.350090	-0.718143	-1.434769
27	1	-3.898279	-2.372851	-1.135454
28	6	-3.464786	-0.675293	1.105175
29	1	-3.150516	-0.733696	2.153439
30	1	-4.499857	-1.051898	1.063512
31	6	-1.958322	-2.222354	-2.032321
32	1	-1.609528	-3.228317	-1.767314
33	1	-2.390345	-2.267478	-3.039251
34	6	-0.004798	-1.409446	-3.228708
35	1	-0.646456	-1.323147	-4.114208
36	1	0.480784	-2.392463	-3.258121
37	6	0.994577	-0.255331	-3.241930
38	1	0.434965	0.680368	-3.296567
39	1	1.600491	-0.349089	-4.158296
40	6	-3.426708	0.768355	0.669250
41	6	-4.519326	1.620915	0.842492
42	1	-5.433630	1.249367	1.295137
43	6	-4.414798	2.946884	0.421112
44	1	-5.247412	3.631015	0.555472
45	6	-3.241966	3.368502	-0.203068
46	1	-3.107912	4.371993	-0.590345
47	6	-2.207726	2.449418	-0.354040
48	6	-0.940729	2.781500	-1.115327
49	7	-2.285461	1.185384	0.103854
50	6	2.529201	1.144464	-1.941743
51	1	1.815193	1.910982	-2.248417
52	1	3.398174	1.183934	-2.613887
53	6	2.940836	1.454677	-0.515646
54	6	4.089077	2.179508	-0.191831
55	1	4.773343	2.496307	-0.972915
56	6	4.333850	2.499343	1.146735
57	1	5.220583	3.065657	1.416101
58	6	3.433537	2.089163	2.129293
59	1	3.570257	2.311218	3.181405
60	6	2.311400	1.366189	1.730023
61	6	1.253442	0.879738	2.715008
62	7	2.088795	1.055352	0.442830
63	8	0.215539	0.320667	2.129859
64	8	1.430140	1.011366	3.912587

65	8	-0.776284	3.891957	-1.592076
66	8	-0.130451	1.760375	-1.207752

E(RB3LYP) = -1715.9122743 Hartrees
Corrección de punto cero = 0.541940 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.337311 Hartrees
Suma de las energías libres y térmicas = -1715.432186 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(δδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.036450	-0.257447	0.011927
2	7	-2.793553	-1.203367	0.081898
3	7	2.022731	-0.811143	-1.772066
4	8	-0.793683	-1.426774	-2.041246
5	8	1.686974	-2.307348	0.618574
6	8	-0.753221	-2.384756	1.530821
7	6	3.044198	-1.760589	-1.257228
8	1	3.647773	-2.173440	-2.079981
9	1	3.721102	-1.204401	-0.605742
10	6	2.451573	-2.888250	-0.440968
11	1	1.806778	-3.555146	-1.032243
12	1	3.268982	-3.492070	-0.025595
13	6	1.424260	-3.238921	1.675404
14	1	2.322826	-3.370626	2.292095
15	1	1.143488	-4.207909	1.241168
16	6	0.272793	-2.690926	2.487754
17	1	-0.074255	-3.451356	3.196678
18	1	0.535844	-1.778591	3.031300
19	6	-2.088344	-2.660045	1.946820
20	1	-2.384369	-1.970306	2.747340
21	1	-2.156926	-3.683409	2.338846
22	6	-2.952019	-2.534326	0.703157
23	1	-2.624283	-3.296320	-0.008316
24	1	-4.005247	-2.746141	0.948212
25	6	-3.150270	-1.214946	-1.355781
26	1	-3.224435	-0.177113	-1.687147
27	1	-4.134765	-1.685377	-1.523587
28	6	-3.616820	-0.223453	0.831635
29	1	-3.439943	-0.382300	1.900451
30	1	-4.691355	-0.402029	0.661103
31	6	-2.131083	-1.934163	-2.242103
32	1	-2.103363	-3.011798	-2.048110
33	1	-2.425759	-1.790690	-3.286311
34	6	-0.054277	-0.981035	-3.211999
35	6	1.416226	-1.340433	-3.022477
36	6	-3.273514	1.206437	0.485515
37	6	-4.173694	2.260669	0.659522
38	1	-5.159205	2.075913	1.076386
39	6	-3.785488	3.545812	0.278058
40	1	-4.461821	4.383992	0.417267
41	6	-2.541371	3.731024	-0.326083
42	1	-2.204789	4.692338	-0.697207
43	6	-1.717508	2.621259	-0.484440
44	6	-0.422269	2.660859	-1.271962
45	7	-2.057865	1.398841	-0.037434
46	6	2.689364	0.507923	-1.965276
47	1	2.001960	1.166014	-2.499757

48	1	3.608125	0.392568	-2.560252
49	6	3.002744	1.146978	-0.623903
50	6	4.106220	1.973960	-0.411004
51	1	4.809795	2.164387	-1.215527
52	6	4.283580	2.556134	0.847499
53	1	5.134328	3.206383	1.028898
54	6	3.366269	2.294801	1.864453
55	1	3.455213	2.716296	2.859089
56	6	2.289345	1.458780	1.576930
57	6	1.209661	1.126592	2.601450
58	7	2.128198	0.901268	0.365898
59	8	0.204797	0.442036	2.095010
60	8	1.335987	1.485342	3.757628
61	8	0.011186	3.714664	-1.707805
62	8	0.089648	1.468254	-1.438753
63	1	1.489507	-2.431668	-2.993103
64	1	1.977048	-1.004203	-3.907591
65	1	-0.431725	-1.504606	-4.096423
66	1	-0.205914	0.095173	-3.322756

E(RB3LYP) = -1715.9071018 Hartrees
Corrección de punto cero = 0.541878 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.332255 Hartrees
Suma de las energías libres y térmicas = -1715.426932 Hartrees

$[Ho(dpa15c5)]^+$ (vacío) Λ(λδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.137731	0.097186	0.009099
2	7	-2.205611	1.754745	-0.747401
3	7	1.710545	0.384980	1.943304
4	8	-0.890743	1.661734	1.790147
5	8	3.056550	1.256800	-0.595651
6	8	0.568231	2.392820	-1.079721
7	6	2.730406	1.463799	1.818322
8	6	3.715371	1.311437	0.659530
9	6	2.958606	2.469745	-1.326769
10	6	1.634328	2.429144	-2.060125
11	6	-0.395050	3.452854	-1.120152
12	6	-1.747777	2.906122	-1.561012
13	6	-2.886552	2.163899	0.509592
14	1	-3.455277	1.303363	0.865653
15	1	-3.606984	2.976098	0.320499
16	6	-3.115395	0.904994	-1.571425
17	1	-2.594535	0.697912	-2.513067
18	1	-4.047913	1.436407	-1.815569
19	6	-1.961591	2.606631	1.646380
20	1	-1.544379	3.608773	1.493239
21	1	-2.547513	2.632640	2.574180
22	6	-0.082334	1.844543	2.971036
23	6	0.851611	0.648912	3.132677
24	6	-3.422509	-0.412003	-0.894043
25	6	-4.624024	-1.100006	-1.061013
26	1	-5.406842	-0.691606	-1.692588
27	6	-4.797653	-2.319451	-0.399609
28	1	-5.721253	-2.877404	-0.522370
29	6	-3.789547	-2.796751	0.436853
30	1	-3.878807	-3.718487	1.000304

31	6	-2.624603	-2.043240	0.561386
32	6	-1.490476	-2.427969	1.500126
33	7	-2.445253	-0.893494	-0.111363
34	6	2.353034	-0.960317	2.077967
35	1	1.639158	-1.608863	2.592213
36	1	3.259903	-0.897142	2.696733
37	6	2.661421	-1.615190	0.742205
38	6	3.710727	-2.518415	0.558116
39	1	4.384624	-2.752157	1.376855
40	6	3.873295	-3.116426	-0.694505
41	1	4.680456	-3.825106	-0.855333
42	6	3.003933	-2.790731	-1.736216
43	1	3.093834	-3.213573	-2.730187
44	6	1.984351	-1.879072	-1.476732
45	6	0.992365	-1.420535	-2.542327
46	7	1.825836	-1.326248	-0.263528
47	8	0.089507	-0.575655	-2.085439
48	8	1.099581	-1.823613	-3.685351
49	8	-1.584981	-3.428297	2.190131
50	8	-0.497596	-1.576205	1.471050
51	1	-2.493271	3.717926	-1.560724
52	1	-1.642694	2.559760	-2.592886
53	1	-0.076717	4.229791	-1.823441
54	1	-0.428970	3.909903	-0.128674
55	1	1.519082	3.307533	-2.703035
56	1	1.554476	1.526124	-2.670680
57	1	2.988337	3.342062	-0.658653
58	1	3.786400	2.555282	-2.045860
59	1	4.422728	2.150461	0.700738
60	1	4.301515	0.393786	0.752607
61	1	2.202824	2.415216	1.697142
62	1	3.312778	1.529167	2.753460
63	1	0.241190	-0.241983	3.291592
64	1	1.460471	0.817118	4.035796
65	1	-0.737851	1.891506	3.849382
66	1	0.448564	2.801624	2.893047

E(RB3LYP) = -1715.906025 Hartrees
Corrección de punto cero = 0.541491 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.331453 Hartrees
Suma de las energías libres y térmicas = -1715.426889 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(λλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.013310	0.146408	0.035150
2	7	-2.385107	1.896276	-0.006729
3	7	1.450908	-0.597080	2.171989
4	8	-1.223833	0.365120	2.209058
5	8	2.038100	1.772592	0.796678
6	8	0.203761	2.825146	-0.598240
7	6	2.169686	0.526174	2.813643
8	6	2.947623	1.371145	1.820005
9	6	2.447969	2.948836	0.090947
10	6	1.509542	3.122988	-1.090730
11	6	-0.881341	3.304143	-1.394394
12	1	-0.997863	2.674882	-2.285687
13	1	-0.685267	4.335321	-1.716773

14	6	-2.085061	3.281153	-0.471186
15	1	-1.840767	3.898919	0.395863
16	1	-2.957830	3.736360	-0.961639
17	6	-2.905627	1.911175	1.383876
18	6	-3.331600	1.300716	-0.978756
19	1	-2.975407	1.568784	-1.980780
20	1	-4.331365	1.751073	-0.868633
21	6	-2.638269	0.657799	2.212016
22	6	-0.723795	-0.250520	3.418045
23	1	-1.513893	-0.856490	3.875076
24	1	-0.463536	0.548714	4.121980
25	6	0.448755	-1.179833	3.103220
26	1	0.061547	-2.075939	2.618443
27	1	0.910509	-1.474085	4.059940
28	6	-3.436893	-0.202923	-0.925842
29	6	-4.616170	-0.859220	-1.285409
30	1	-5.495983	-0.284663	-1.558635
31	6	-4.640308	-2.254244	-1.291922
32	1	-5.543476	-2.785550	-1.577280
33	6	-3.496417	-2.950136	-0.908030
34	1	-3.449501	-4.032156	-0.865356
35	6	-2.366720	-2.221019	-0.544780
36	6	-1.116687	-2.909366	-0.028727
37	7	-2.329844	-0.873918	-0.571710
38	6	2.396707	-1.661705	1.722619
39	1	1.832792	-2.597607	1.685669
40	1	3.209522	-1.788635	2.452536
41	6	2.960093	-1.459701	0.327406
42	6	4.179675	-2.011890	-0.073852
43	1	4.813095	-2.522626	0.645112
44	6	4.556712	-1.912953	-1.415475
45	1	5.498012	-2.341075	-1.747498
46	6	3.713804	-1.271643	-2.323843
47	1	3.948949	-1.176990	-3.377772
48	6	2.519161	-0.738626	-1.846284
49	6	1.514961	-0.027890	-2.749396
50	7	2.173483	-0.824100	-0.550871
51	8	0.405737	0.310665	-2.131264
52	8	1.798743	0.192388	-3.913624
53	8	-1.089218	-4.125139	0.075003
54	8	-0.171778	-2.072649	0.300094
55	1	1.432487	1.175795	3.293270
56	1	2.851473	0.161915	3.599003
57	1	3.792168	0.830664	1.374548
58	1	3.342985	2.254256	2.339138
59	1	-2.959783	0.867414	3.238708
60	1	-3.178049	-0.222916	1.852926
61	1	-3.990337	2.107876	1.405766
62	1	-2.417970	2.740157	1.903211
63	1	1.559457	4.159429	-1.448895
64	1	1.757598	2.454885	-1.921308
65	1	2.385541	3.806711	0.773589
66	1	3.483666	2.848251	-0.258824

E(RB3LYP) = -1715.9094183 Hartrees
Corrección de punto cero = 0.542287 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.334210 Hartrees
Suma de las energías libres y térmicas = -1715.428574 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(δλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.009032	-0.257250	-0.011954
2	7	2.758796	-1.475410	-0.055235
3	7	-1.912464	-0.523560	1.973740
4	8	0.981475	-0.916609	2.229495
5	8	-1.755240	-2.321051	-0.197473
6	8	0.534016	-2.488106	-1.401294
7	6	-2.953895	-1.550132	1.702403
8	1	-3.461591	-1.850697	2.631508
9	1	-3.706639	-1.101643	1.050965
10	6	-2.407814	-2.770709	0.994125
11	1	-1.695468	-3.343182	1.605974
12	1	-3.241888	-3.435894	0.736711
13	6	-1.630026	-3.352339	-1.186170
14	6	-0.594400	-2.891013	-2.189141
15	6	1.822769	-2.821718	-1.913327
16	1	2.105298	-2.120629	-2.708599
17	1	1.806683	-3.832120	-2.341565
18	6	2.762159	-2.800684	-0.720597
19	1	2.400671	-3.546653	-0.008387
20	1	3.775512	-3.102260	-1.031007
21	6	3.150152	-1.588999	1.374058
22	6	3.642104	-0.574262	-0.828655
23	1	3.476900	-0.775188	-1.892860
24	1	4.701341	-0.808411	-0.631929
25	6	2.401225	-0.675704	2.341029
26	6	0.222235	-0.321818	3.310961
27	6	-1.206276	-0.841156	3.241609
28	6	3.393969	0.895591	-0.593854
29	6	4.394888	1.845404	-0.818354
30	1	5.380536	1.529480	-1.146784
31	6	4.107005	3.193883	-0.611692
32	1	4.864654	3.950332	-0.793678
33	6	2.847332	3.549265	-0.131135
34	1	2.570138	4.571798	0.098138
35	6	1.919013	2.538156	0.095671
36	6	0.592981	2.809343	0.778021
37	7	2.170133	1.241310	-0.174518
38	6	-2.585377	0.805150	2.014173
39	1	-1.870830	1.542607	2.385148
40	1	-3.450777	0.778488	2.693598
41	6	-3.010769	1.232830	0.621684
42	6	-4.135021	2.021159	0.374331
43	1	-4.783425	2.321217	1.191749
44	6	-4.402564	2.425117	-0.936946
45	1	-5.271268	3.041756	-1.148037
46	6	-3.545904	2.037112	-1.966228
47	1	-3.699002	2.327715	-2.999203
48	6	-2.442160	1.251800	-1.639575
49	6	-1.407425	0.815656	-2.669365
50	7	-2.203178	0.852213	-0.380864
51	8	-0.348335	0.247649	-2.129607
52	8	-1.608992	0.998158	-3.855673
53	8	0.250921	3.950595	1.039434
54	8	-0.048442	1.708844	1.071864
55	1	-1.169054	-1.930511	3.339251

56	1	-1.763621	-0.458786	4.110505
57	1	0.664414	-0.634358	4.264998
58	1	0.274528	0.767244	3.223403
59	1	2.721167	-0.928782	3.360029
60	1	2.601593	0.385292	2.168663
61	1	4.228147	-1.407812	1.507501
62	1	2.961157	-2.617733	1.692858
63	1	-0.326780	-3.720927	-2.852884
64	1	-0.934369	-2.044426	-2.792786
65	1	-1.292911	-4.278154	-0.701426
66	1	-2.601405	-3.531315	-1.664921

E(RB3LYP) = -1715.9059945 Hartrees
Corrección de punto cero = 0.542029 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.331044 Hartrees
Suma de las energías libres y térmicas = -1715.425932 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	0.034288	-0.119393	0.033056
2	7	2.611865	-1.414091	-0.346383
3	7	-1.826000	-0.489942	2.002549
4	8	0.917680	-1.410954	2.009649
5	8	-1.940682	-1.824896	-0.405657
6	8	0.314746	-2.580590	-1.441342
7	6	-2.733671	-1.657591	1.807962
8	1	-2.891708	-2.194586	2.753794
9	1	-3.707240	-1.280067	1.485187
10	6	-2.248406	-2.626574	0.734283
11	1	-1.365590	-3.201796	1.045064
12	1	-3.048693	-3.338330	0.493958
13	6	-2.032996	-2.429892	-1.697991
14	6	-0.803598	-3.277405	-1.990574
15	6	1.566508	-2.903083	-2.047790
16	1	1.730501	-2.247242	-2.912214
17	1	1.566503	-3.941674	-2.401938
18	6	2.628936	-2.754932	-0.975201
19	1	2.423864	-3.502883	-0.205777
20	1	3.622868	-2.984761	-1.391156
21	6	3.138297	-1.487186	1.036983
22	1	3.346370	-0.471295	1.377549
23	1	4.086280	-2.049508	1.077449
24	6	3.404858	-0.481040	-1.185355
25	1	3.020477	-0.553051	-2.209424
26	1	4.463606	-0.786159	-1.217916
27	6	2.164726	-2.128228	2.021924
28	1	1.971257	-3.185900	1.801912
29	1	2.602042	-2.069005	3.026264
30	6	0.068625	-1.677417	3.145211
31	1	0.672574	-1.641859	4.060114
32	1	-0.346990	-2.689855	3.054426
33	6	-1.006842	-0.602414	3.232547
34	1	-0.515468	0.360992	3.381810
35	1	-1.630068	-0.814813	4.116509
36	6	3.303161	0.953738	-0.721300
37	6	4.322300	1.883092	-0.936488
38	1	5.226754	1.590708	-1.461166

39	6	4.158524	3.185318	-0.460157
40	1	4.933269	3.928040	-0.626079
41	6	3.008958	3.508580	0.259399
42	1	2.840511	4.487983	0.692247
43	6	2.047489	2.519000	0.444536
44	6	0.810258	2.735387	1.298273
45	7	2.180008	1.281409	-0.067796
46	6	-2.618835	0.777381	2.022429
47	1	-1.972526	1.557318	2.431562
48	1	-3.499924	0.677511	2.671817
49	6	-3.025967	1.222939	0.631277
50	6	-4.230164	1.873505	0.356406
51	1	-4.961212	2.027762	1.144105
52	6	-4.470802	2.330827	-0.942960
53	1	-5.398990	2.845560	-1.173444
54	6	-3.517875	2.116302	-1.938101
55	1	-3.654824	2.441565	-2.963033
56	6	-2.345270	1.448194	-1.590035
57	6	-1.249097	1.121916	-2.601936
58	7	-2.118982	1.024998	-0.337257
59	8	-0.213839	0.509013	-2.068677
60	8	-1.404216	1.406370	-3.775633
61	8	0.614238	3.813460	1.833313
62	8	0.066301	1.663540	1.390858
63	1	-0.866510	-4.275961	-1.534729
64	1	-0.699212	-3.399845	-3.075796
65	1	-2.089172	-1.593768	-2.396642
66	1	-2.952804	-3.022416	-1.777174

E(RB3LYP) = -1715.9084236 Hartrees
Corrección de punto cero = 0.541482 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.333743 Hartrees
Suma de las energías libres y térmicas = -1715.429140 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(λλ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.109389	0.113819	-0.022033
2	7	-2.181947	1.817984	-0.739356
3	7	1.648150	0.238409	2.003360
4	8	-0.898222	1.610679	1.790352
5	8	3.093631	1.298854	-0.399104
6	8	0.643238	2.494045	-0.840713
7	6	2.662807	1.329120	2.007866
8	6	3.697639	1.267235	0.884591
9	6	3.029257	2.560328	-1.047947
10	6	1.719316	2.599658	-1.805710
11	6	-0.373405	3.505575	-0.899169
12	6	-1.630701	2.940398	-1.538980
13	6	-2.829879	2.328744	0.508832
14	6	-3.113581	1.020611	-1.576961
15	1	-2.607618	0.822065	-2.529173
16	1	-4.031997	1.583791	-1.802340
17	6	-2.340164	1.690534	1.815284
18	6	-0.203676	1.602132	3.064111
19	6	0.734237	0.398983	3.170833
20	6	-3.448625	-0.304052	-0.933310
21	6	-4.671307	-0.953324	-1.107173

22	1	-5.453876	-0.495660	-1.704429
23	6	-4.864164	-2.198365	-0.502887
24	1	-5.804261	-2.726574	-0.631970
25	6	-3.848783	-2.742657	0.282410
26	1	-3.946683	-3.691407	0.797545
27	6	-2.664097	-2.023601	0.419814
28	6	-1.525255	-2.485102	1.314803
29	7	-2.467410	-0.842597	-0.193550
30	6	2.296980	-1.109689	2.053311
31	1	1.575913	-1.799621	2.498366
32	1	3.186374	-1.089226	2.699555
33	6	2.648524	-1.662685	0.682001
34	6	3.704199	-2.551679	0.466750
35	1	4.350512	-2.846038	1.288192
36	6	3.909432	-3.056398	-0.820079
37	1	4.722190	-3.752651	-1.005138
38	6	3.075619	-2.653786	-1.864135
39	1	3.199805	-3.002783	-2.882772
40	6	2.047483	-1.761640	-1.573209
41	6	1.092818	-1.222961	-2.635821
42	7	1.847630	-1.299523	-0.328226
43	8	0.175897	-0.408463	-2.149486
44	8	1.237096	-1.542868	-3.800403
45	8	-1.623453	-3.527123	1.939691
46	8	-0.523313	-1.644091	1.331121
47	1	-2.375815	3.740736	-1.676338
48	1	-1.372395	2.553602	-2.529054
49	1	-0.016411	4.368420	-1.470967
50	1	-0.553602	3.836517	0.127579
51	1	1.627767	3.536407	-2.364763
52	1	1.640901	1.760032	-2.501877
53	1	3.059385	3.383052	-0.320329
54	1	3.872437	2.679750	-1.743694
55	1	4.394706	2.105570	1.015482
56	1	4.289276	0.349619	0.937574
57	1	2.132552	2.284076	1.937634
58	1	3.204777	1.324117	2.969220
59	1	0.130835	-0.508104	3.226114
60	1	1.301770	0.497298	4.110935
61	1	-0.931163	1.542300	3.879582
62	1	0.321558	2.558663	3.149061
63	1	-2.657012	2.323676	2.651572
64	1	-2.748130	0.685920	1.962966
65	1	-3.917563	2.191374	0.456877
66	1	-2.657148	3.406744	0.572175

E(RB3LYP) = -1715.9019841 Hartrees
Corrección de punto cero = 0.541658 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.327312 Hartrees
Suma de las energías libres y térmicas = -1715.422507 Hartrees

[Ho(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	67	-0.038708	0.115626	-0.016506
2	7	-2.577306	1.463080	-0.507762
3	7	1.704602	0.207187	2.080624
4	8	-1.040308	1.143638	2.005353

5	8	1.938072	1.944782	-0.073858
6	8	-0.233298	2.893013	-1.129357
7	6	2.568598	1.408528	2.134743
8	6	3.085397	1.817386	0.765402
9	6	2.102474	2.705685	-1.280754
10	6	0.940806	3.673711	-1.322694
11	6	-1.403926	3.668727	-0.930546
12	6	-2.589927	2.768071	-1.218736
13	6	-3.148274	1.553524	0.860756
14	1	-3.499736	0.559221	1.143793
15	1	-4.022829	2.224869	0.880076
16	6	-3.372944	0.522627	-1.348170
17	1	-2.928401	0.540430	-2.349633
18	1	-4.415038	0.865784	-1.447376
19	6	-2.184239	2.016993	1.952933
20	1	-1.841095	3.048424	1.815715
21	1	-2.714504	1.964117	2.912093
22	6	-0.295667	1.213367	3.240713
23	1	-0.978238	1.018551	4.077120
24	1	0.095795	2.231877	3.357235
25	6	0.799789	0.147270	3.257263
26	1	0.327629	-0.836185	3.245101
27	1	1.352596	0.253342	4.204967
28	6	-3.347922	-0.897525	-0.845841
29	6	-4.424600	-1.767880	-1.025993
30	1	-5.326784	-1.422427	-1.521267
31	6	-4.318536	-3.079218	-0.559459
32	1	-5.138930	-3.777199	-0.697771
33	6	-3.159806	-3.468013	0.109530
34	1	-3.024368	-4.458772	0.527852
35	6	-2.139675	-2.532653	0.262751
36	6	-0.884638	-2.835210	1.055602
37	7	-2.220759	-1.282812	-0.230094
38	6	2.529664	-1.031619	1.976672
39	1	1.905690	-1.867971	2.299347
40	1	3.401840	-0.972747	2.644277
41	6	2.971210	-1.340981	0.556746
42	6	4.146061	-2.038236	0.265076
43	1	4.822214	-2.329577	1.063061
44	6	4.428237	-2.361051	-1.065025
45	1	5.334116	-2.908102	-1.309481
46	6	3.543223	-1.976310	-2.072626
47	1	3.711949	-2.199014	-3.119970
48	6	2.394901	-1.278687	-1.705405
49	6	1.353351	-0.809542	-2.719411
50	7	2.131612	-0.975242	-0.423293
51	8	0.310618	-0.231765	-2.161881
52	8	1.548670	-0.978905	-3.908436
53	8	-0.734608	-3.924841	1.583415
54	8	-0.067365	-1.818282	1.112768
55	1	1.036828	4.415769	-0.516022
56	1	0.899898	4.201688	-2.285668
57	1	2.084511	2.026899	-2.139133
58	1	3.054552	3.246531	-1.271827
59	1	-3.526971	3.313573	-1.022742
60	1	-2.558281	2.551260	-2.289022
61	1	-1.409483	4.096716	0.082104
62	1	-1.435101	4.509331	-1.638317
63	1	3.597505	2.784673	0.849988
64	1	3.790066	1.092108	0.344109

65	1	3.414774	1.255868	2.822697
66	1	1.980615	2.243626	2.523084

E(RB3LYP) = -1715.9077935 Hartrees
Corrección de punto cero = 0.541888 Hartrees
Suma de las entalpías electrónicas y térmicas = -1715.332804 Hartrees
Suma de las energías libres y térmicas = -1715.428550 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	0.060405	-0.170260	0.088028
2	7	2.510356	-1.519278	-0.300962
3	7	-1.795312	-0.344883	2.049588
4	8	0.928064	-1.267446	2.100315
5	8	-1.967006	-2.021311	-0.186161
6	8	0.159391	-2.539181	-1.416203
7	6	-2.665635	-1.543329	2.010079
8	6	-3.141269	-1.867383	0.606169
9	6	-2.210237	-2.353714	-1.556295
10	6	-0.983503	-3.100924	-2.056821
11	6	1.391298	-2.955596	-1.995176
12	1	1.620237	-2.327382	-2.865469
13	1	1.321002	-3.997382	-2.335709
14	6	2.437376	-2.872040	-0.899926
15	1	2.154044	-3.582377	-0.119214
16	1	3.420559	-3.185483	-1.285894
17	6	3.089059	-1.590410	1.062419
18	1	3.401189	-0.585923	1.354347
19	1	3.983832	-2.234048	1.085004
20	6	3.327838	-0.648771	-1.183808
21	1	2.920197	-0.728250	-2.197297
22	1	4.370853	-1.001820	-1.224156
23	6	2.101827	-2.100906	2.105301
24	1	1.799919	-3.142100	1.934975
25	1	2.577400	-2.043756	3.091952
26	6	0.120478	-1.394402	3.290031
27	1	0.756296	-1.234071	4.169345
28	1	-0.271000	-2.418285	3.340447
29	6	-0.974383	-0.332279	3.287242
30	1	-0.503004	0.649406	3.346912
31	1	-1.591064	-0.479185	4.188787
32	6	3.286986	0.798157	-0.756228
33	6	4.328756	1.691289	-1.012659
34	1	5.217017	1.357790	-1.540419
35	6	4.207262	3.011464	-0.574830
36	1	5.000764	3.726405	-0.771283
37	6	3.072593	3.390734	0.141367
38	1	2.933590	4.389477	0.539148
39	6	2.086780	2.434341	0.366050
40	6	0.850957	2.708656	1.198928
41	7	2.183101	1.175907	-0.098581
42	6	-2.608511	0.900395	1.945625
43	1	-2.013852	1.715375	2.365051
44	1	-3.532770	0.811370	2.535233
45	6	-2.928772	1.295871	0.516232
46	6	-4.059022	2.043513	0.176232
47	1	-4.791592	2.302273	0.934650

48	6	-4.222166	2.461046	-1.147040
49	1	-5.092324	3.047402	-1.427473
50	6	-3.261027	2.124028	-2.100477
51	1	-3.332066	2.424634	-3.139523
52	6	-2.163779	1.373045	-1.687260
53	6	-1.039149	0.958577	-2.631400
54	7	-2.018629	0.967773	-0.413230
55	8	-0.054842	0.345357	-2.016864
56	8	-1.129160	1.194475	-3.823053
57	8	0.672893	3.804144	1.704448
58	8	0.078009	1.659100	1.306703
59	1	-1.041543	-4.168081	-1.801129
60	1	-0.909237	-3.002722	-3.147323
61	1	-2.388039	-1.437091	-2.128999
62	1	-3.095711	-2.995217	-1.643219
63	1	-2.093515	-2.402700	2.368212
64	1	-3.531474	-1.423302	2.679667
65	1	-3.787251	-1.084645	0.191651
66	1	-3.709143	-2.807766	0.618037

E(RB3LYP) = -1718.2176357 Hartrees
Corrección de punto cero = 0.542314 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.642345 Hartrees
Suma de las energías libres y térmicas = -1717.737071 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	0.057304	-0.143675	0.104795
2	7	2.455426	-1.618831	-0.263830
3	7	-1.768172	-0.140306	2.074570
4	8	0.900721	-1.180733	2.141843
5	8	-2.101821	-1.866871	-0.111843
6	8	0.025699	-2.717413	-1.234477
7	6	-2.666198	-1.316573	2.129305
8	6	-3.212956	-1.712609	0.769294
9	6	-2.323386	-2.831858	-1.143629
10	6	-1.126947	-2.791821	-2.072549
11	6	1.240662	-3.028700	-1.904895
12	1	1.411835	-2.319423	-2.725206
13	1	1.189477	-4.040920	-2.330703
14	6	2.322668	-2.977177	-0.844691
15	1	2.041053	-3.674904	-0.051631
16	1	3.283446	-3.322430	-1.256881
17	6	3.026169	-1.686165	1.102706
18	1	3.398471	-0.694236	1.367397
19	1	3.880276	-2.381685	1.147624
20	6	3.320113	-0.811447	-1.160229
21	1	2.926000	-0.909838	-2.177259
22	1	4.347740	-1.209099	-1.172870
23	6	2.007567	-2.103969	2.156021
24	1	1.623807	-3.119828	1.999487
25	1	2.488992	-2.069474	3.140595
26	6	0.127077	-1.174905	3.360819
27	1	0.796299	-0.968196	4.204840
28	1	-0.301713	-2.173787	3.508423
29	6	-0.926909	-0.072603	3.297919
30	1	-0.419906	0.892762	3.282230

31	1	-1.534714	-0.133218	4.215214
32	6	3.336458	0.650232	-0.788148
33	6	4.420378	1.483051	-1.073409
34	1	5.297343	1.084572	-1.574361
35	6	4.355154	2.826537	-0.700960
36	1	5.182168	3.495053	-0.921094
37	6	3.230309	3.289466	-0.019511
38	1	3.130646	4.311686	0.327069
39	6	2.200775	2.389525	0.238843
40	6	0.971429	2.763956	1.040175
41	7	2.243657	1.105579	-0.161380
42	6	-2.551777	1.118230	1.903113
43	1	-1.931828	1.941381	2.265723
44	1	-3.470319	1.088383	2.507071
45	6	-2.879818	1.426241	0.453766
46	6	-4.003757	2.161830	0.068533
47	1	-4.725419	2.487987	0.811259
48	6	-4.175692	2.476311	-1.281908
49	1	-5.040263	3.052146	-1.598887
50	6	-3.234434	2.044495	-2.217496
51	1	-3.320206	2.255498	-3.277290
52	6	-2.142257	1.314151	-1.757275
53	6	-1.052401	0.778419	-2.677854
54	7	-1.983800	1.019736	-0.456143
55	8	-0.059989	0.209975	-2.028387
56	8	-1.170100	0.877545	-3.886134
57	8	0.838577	3.890778	1.486693
58	8	0.149485	1.757829	1.192330
59	1	-2.098121	-2.168102	2.511354
60	1	-3.500286	-1.139849	2.827002
61	1	-3.914115	-0.975668	0.359889
62	1	-3.746769	-2.666349	0.872682
63	1	-1.105688	-3.708425	-2.677617
64	1	-1.151373	-1.926973	-2.743549
65	1	-2.426941	-3.823193	-0.681847
66	1	-3.242247	-2.602746	-1.699447

E(RB3LYP) = -1718.2207713 Hartrees
Corrección de punto cero = 0.542597 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.645365 Hartrees
Suma de las energías libres y térmicas = -1717.739373 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.038306	-0.107326	-0.060939
2	7	-2.456816	-1.626763	0.291197
3	7	1.886660	-0.082205	-2.006357
4	8	-0.737380	-1.306918	-2.052438
5	8	2.122929	-1.967156	0.076915
6	8	-0.051249	-2.588964	1.343221
7	6	2.970748	-1.100778	-1.967165
8	1	3.295643	-1.364729	-2.984865
9	1	3.828629	-0.648076	-1.464254
10	6	2.631063	-2.360900	-1.194030
11	1	1.895751	-3.001864	-1.700497
12	1	3.551346	-2.948151	-1.072476
13	6	2.219127	-3.009096	1.055406

14	1	3.223097	-3.018162	1.499034
15	1	2.033320	-3.978174	0.574176
16	6	1.150265	-2.757829	2.094355
17	1	1.073628	-3.627524	2.759798
18	1	1.345162	-1.867767	2.701688
19	6	-1.254313	-2.893991	2.037903
20	1	-1.449350	-2.138879	2.809767
21	1	-1.173535	-3.875683	2.524897
22	6	-2.324860	-2.940880	0.965176
23	1	-2.022138	-3.690475	0.229713
24	1	-3.288169	-3.267090	1.385831
25	6	-2.924701	-1.781937	-1.105291
26	1	-3.287970	-0.812442	-1.454244
27	1	-3.765907	-2.491794	-1.173781
28	6	-3.392211	-0.800213	1.090427
29	1	-3.065077	-0.852686	2.134773
30	1	-4.412083	-1.216498	1.053505
31	6	-1.830308	-2.249850	-2.060251
32	1	-1.441681	-3.243189	-1.804999
33	1	-2.250085	-2.297373	-3.071912
34	6	0.096304	-1.350951	-3.234278
35	1	-0.546451	-1.277765	-4.119799
36	1	0.613002	-2.317533	-3.269016
37	6	1.058257	-0.166228	-3.231179
38	1	0.471994	0.752428	-3.287263
39	1	1.678778	-0.236941	-4.139732
40	6	-3.410790	0.645305	0.665131
41	6	-4.525602	1.463378	0.863038
42	1	-5.420080	1.061119	1.328798
43	6	-4.468535	2.794632	0.449899
44	1	-5.319296	3.451959	0.602864
45	6	-3.318507	3.257279	-0.188290
46	1	-3.220846	4.268066	-0.567455
47	6	-2.260367	2.370732	-0.361410
48	6	-1.008373	2.739816	-1.125344
49	7	-2.293455	1.100638	0.083818
50	6	2.518258	1.264418	-1.870296
51	1	1.792173	2.012935	-2.191831
52	1	3.411269	1.346422	-2.505588
53	6	2.860886	1.556238	-0.422374
54	6	3.970212	2.308597	-0.032559
55	1	4.674926	2.666925	-0.776563
56	6	4.150108	2.600393	1.322646
57	1	5.006256	3.186995	1.642704
58	6	3.224807	2.135522	2.256724
59	1	3.312046	2.333139	3.318952
60	6	2.144176	1.389439	1.792457
61	6	1.060863	0.841418	2.713114
62	7	1.983936	1.105521	0.489807
63	8	0.066141	0.276710	2.062040
64	8	1.179998	0.933345	3.921452
65	8	-0.869134	3.853035	-1.602250
66	8	-0.172050	1.738138	-1.217395

E(RB3LYP) = -1718.214945 Hartrees
Corrección de punto cero = 0.542326 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.639669 Hartrees
Suma de las energías libres y térmicas = -1717.734480 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(δδ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.032563	-0.248701	-0.020975
2	7	-2.761316	-1.224737	0.064338
3	7	2.061968	-0.773974	-1.738736
4	8	-0.731406	-1.423723	-2.026270
5	8	1.719482	-2.260416	0.642982
6	8	-0.724256	-2.414394	1.508125
7	6	3.092934	-1.706354	-1.212130
8	1	3.712773	-2.109343	-2.027526
9	1	3.753083	-1.139616	-0.552400
10	6	2.504923	-2.838501	-0.401372
11	1	1.876650	-3.516000	-0.998431
12	1	3.323984	-3.430252	0.027940
13	6	1.473041	-3.186938	1.707758
14	1	2.365245	-3.278006	2.340859
15	1	1.235201	-4.170784	1.281677
16	6	0.287538	-2.673431	2.490554
17	1	-0.047394	-3.442014	3.197213
18	1	0.505659	-1.749621	3.034469
19	6	-2.058822	-2.664070	1.936804
20	1	-2.342551	-1.953982	2.723956
21	1	-2.138308	-3.678521	2.350245
22	6	-2.923947	-2.550882	0.694900
23	1	-2.598313	-3.320486	-0.009200
24	1	-3.977968	-2.756688	0.940752
25	6	-3.101219	-1.251993	-1.376124
26	1	-3.187550	-0.218819	-1.719205
27	1	-4.075287	-1.740240	-1.553327
28	6	-3.596900	-0.245472	0.799586
29	1	-3.434192	-0.401012	1.870928
30	1	-4.668589	-0.426372	0.614012
31	6	-2.056387	-1.964064	-2.236289
32	1	-2.007039	-3.036936	-2.022733
33	1	-2.337258	-1.844401	-3.286980
34	6	0.008337	-0.988361	-3.202734
35	6	1.484357	-1.313165	-2.997433
36	6	-3.250310	1.182783	0.455801
37	6	-4.144888	2.241401	0.635315
38	1	-5.129416	2.060231	1.056067
39	6	-3.752564	3.525249	0.254986
40	1	-4.424401	4.366303	0.398444
41	6	-2.509336	3.705949	-0.353225
42	1	-2.169683	4.666575	-0.723408
43	6	-1.692689	2.592148	-0.515609
44	6	-0.399308	2.617478	-1.302082
45	7	-2.036663	1.370043	-0.070993
46	6	2.712327	0.554955	-1.912845
47	1	2.036759	1.201739	-2.474532
48	1	3.655537	0.454076	-2.470902
49	6	2.963283	1.194395	-0.558596
50	6	4.042157	2.040034	-0.298307
51	1	4.770888	2.250186	-1.075031
52	6	4.163210	2.614657	0.970289
53	1	4.994766	3.278575	1.187546
54	6	3.214603	2.328211	1.951255
55	1	3.259714	2.742702	2.951790

56	6	2.164774	1.475757	1.617095
57	6	1.052222	1.111590	2.592193
58	7	2.057757	0.925035	0.396862
59	8	0.083886	0.413748	2.034286
60	8	1.121004	1.455930	3.757388
61	8	0.050980	3.661487	-1.743702
62	8	0.096919	1.416351	-1.462115
63	1	1.583178	-2.402324	-2.968509
64	1	2.046739	-0.962765	-3.875943
65	1	-0.353376	-1.540188	-4.076179
66	1	-0.165975	0.081042	-3.336962

E(RB3LYP) = -1718.2094663 Hartrees
Corrección de punto cero = 0.542236 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.634313 Hartrees
Suma de las energías libres y térmicas = -1717.729084 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	0.176246	-0.083350	0.050560
2	7	2.003072	-1.808882	-0.876853
3	7	-1.711644	-0.413335	1.887369
4	8	0.806690	-1.787247	1.674437
5	8	-3.415857	-0.956446	-0.632489
6	8	-0.858882	-2.174590	-1.071169
7	6	-2.759591	-1.461492	1.703317
8	6	-3.869690	-1.170384	0.689551
9	6	-3.248414	-2.094444	-1.463414
10	6	-1.874355	-2.026978	-2.099013
11	6	0.019683	-3.300927	-1.210836
12	6	1.380010	-2.848773	-1.729774
13	6	2.712885	-2.373033	0.302332
14	1	3.391773	-1.602380	0.670534
15	1	3.329737	-3.238741	0.013672
16	6	2.946749	-0.987208	-1.691703
17	1	2.403354	-0.667624	-2.587360
18	1	3.817387	-1.577960	-2.013503
19	6	1.810183	-2.792017	1.465616
20	1	1.323496	-3.760683	1.301407
21	1	2.425231	-2.882283	2.369894
22	6	0.001873	-1.989201	2.856003
23	6	-0.878242	-0.763794	3.072324
24	6	3.388297	0.246649	-0.935676
25	6	4.627412	0.863271	-1.105390
26	1	5.352908	0.456216	-1.802845
27	6	4.913344	2.011573	-0.360139
28	1	5.869176	2.512629	-0.481604
29	6	3.974996	2.493663	0.552210
30	1	4.152234	3.363700	1.174062
31	6	2.764155	1.815611	0.669119
32	6	1.676445	2.210151	1.656418
33	7	2.483243	0.732283	-0.073451
34	6	-2.306821	0.944356	2.080215
35	1	-1.581901	1.537067	2.644626
36	1	-3.229804	0.891116	2.674563
37	6	-2.546764	1.671848	0.769676
38	6	-3.548113	2.627973	0.592589

39	1	-4.241623	2.852629	1.397337
40	6	-3.637618	3.291724	-0.634003
41	1	-4.408041	4.041377	-0.789004
42	6	-2.741139	2.981244	-1.657075
43	1	-2.772270	3.457905	-2.630063
44	6	-1.772611	2.013978	-1.405676
45	6	-0.752876	1.565530	-2.446553
46	7	-1.686793	1.392867	-0.218309
47	8	0.082087	0.652256	-1.991958
48	8	-0.780889	2.030622	-3.570572
49	8	1.854835	3.137089	2.426082
50	8	0.614387	1.446581	1.567807
51	1	2.041923	-3.722268	-1.845313
52	1	1.230642	-2.415434	-2.722670
53	1	-0.408553	-4.031019	-1.905769
54	1	0.082621	-3.785320	-0.235314
55	1	-1.757017	-2.818456	-2.846419
56	1	-1.716193	-1.062484	-2.585084
57	1	-3.355122	-3.027728	-0.893837
58	1	-4.013143	-2.087141	-2.253288
59	1	-4.576956	-2.011248	0.733449
60	1	-4.428717	-0.273181	0.967892
61	1	-2.257247	-2.389704	1.415243
62	1	-3.256935	-1.645159	2.671338
63	1	-0.231676	0.091347	3.277368
64	1	-1.503541	-0.948288	3.960716
65	1	0.663000	-2.104301	3.723484
66	1	-0.571148	-2.917312	2.737611

E(RB3LYP) = -1718.2123353 Hartrees
Corrección de punto cero = 0.542220 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.637337 Hartrees
Suma de las energías libres y térmicas = -1717.731320 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.019146	0.112790	0.055463
2	7	-2.298909	1.940871	0.038415
3	7	1.459681	-0.659192	2.142304
4	8	-1.187076	0.317955	2.196281
5	8	2.100489	1.713882	0.828011
6	8	0.301878	2.810300	-0.554993
7	6	2.189212	0.436397	2.819431
8	6	2.992037	1.287582	1.852770
9	6	2.548290	2.874034	0.122936
10	6	1.610119	3.075768	-1.053968
11	6	-0.772217	3.329254	-1.338406
12	1	-0.912025	2.714878	-2.236307
13	1	-0.550697	4.359687	-1.647093
14	6	-1.968110	3.325268	-0.406295
15	1	-1.700260	3.922202	0.468375
16	1	-2.834109	3.809352	-0.880707
17	6	-2.813760	1.950203	1.429940
18	6	-3.265040	1.387238	-0.938411
19	1	-2.905844	1.661129	-1.937515
20	1	-4.252251	1.861380	-0.815828
21	6	-2.588035	0.671265	2.228814

22	6	-0.705837	-0.336098	3.393890
23	1	-1.507580	-0.947003	3.823122
24	1	-0.447458	0.441758	4.121922
25	6	0.463063	-1.263610	3.064216
26	1	0.074873	-2.150716	2.564963
27	1	0.926621	-1.573322	4.015018
28	6	-3.406883	-0.112897	-0.908350
29	6	-4.598166	-0.737214	-1.285794
30	1	-5.461797	-0.138422	-1.558585
31	6	-4.655324	-2.130818	-1.310237
32	1	-5.568490	-2.637032	-1.608977
33	6	-3.530603	-2.858352	-0.927446
34	1	-3.509264	-3.941642	-0.898572
35	6	-2.387575	-2.159646	-0.548529
36	6	-1.153094	-2.875711	-0.039862
37	7	-2.318949	-0.813670	-0.555086
38	6	2.400601	-1.709585	1.652579
39	1	1.846065	-2.651138	1.618065
40	1	3.235214	-1.839742	2.356525
41	6	2.920404	-1.478946	0.245221
42	6	4.123615	-2.026126	-0.208877
43	1	4.778777	-2.554043	0.477469
44	6	4.455539	-1.901178	-1.560139
45	1	5.383772	-2.324890	-1.932177
46	6	3.583383	-1.241702	-2.427205
47	1	3.781631	-1.129188	-3.486963
48	6	2.407905	-0.715910	-1.898154
49	6	1.367310	0.006502	-2.746978
50	7	2.107790	-0.822493	-0.592881
51	8	0.283327	0.326857	-2.076041
52	8	1.600045	0.249801	-3.917738
53	8	-1.147542	-4.090970	0.068425
54	8	-0.187887	-2.056931	0.278992
55	1	1.457481	1.087318	3.305666
56	1	2.854647	0.040391	3.603324
57	1	3.836619	0.742607	1.411151
58	1	3.393146	2.156284	2.392165
59	1	-2.881664	0.872803	3.265269
60	1	-3.170055	-0.179020	1.863073
61	1	-3.890252	2.186868	1.461657
62	1	-2.292626	2.749957	1.962433
63	1	1.685169	4.111048	-1.411525
64	1	1.840100	2.405162	-1.888091
65	1	2.515852	3.734940	0.804250
66	1	3.579567	2.740195	-0.229670

E(RB3LYP) = -1718.2125413 Hartrees
Corrección de punto cero = 0.542611 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.637071 Hartrees
Suma de las energías libres y térmicas = -1717.731350 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(δλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	-0.016277	-0.236094	0.016830
2	7	2.743640	-1.496986	-0.050691
3	7	-1.933376	-0.508194	1.957421
4	8	0.942883	-0.916565	2.207689

5	8	-1.765504	-2.279787	-0.213602
6	8	0.514946	-2.480353	-1.399016
7	6	-2.975855	-1.532491	1.682348
8	1	-3.484131	-1.836275	2.609883
9	1	-3.728387	-1.082255	1.031722
10	6	-2.423909	-2.745272	0.968128
11	1	-1.713764	-3.321740	1.578765
12	1	-3.254315	-3.410045	0.698518
13	6	-1.664390	-3.294037	-1.222552
14	6	-0.608649	-2.844535	-2.207939
15	6	1.800190	-2.780798	-1.936964
16	1	2.072131	-2.040758	-2.700020
17	1	1.787453	-3.770833	-2.410913
18	6	2.744721	-2.803775	-0.749815
19	1	2.382662	-3.569496	-0.059306
20	1	3.756691	-3.098306	-1.070762
21	6	3.105817	-1.645408	1.379887
22	6	3.644736	-0.587218	-0.789296
23	1	3.516349	-0.783827	-1.859286
24	1	4.698769	-0.815218	-0.559046
25	6	2.369239	-0.721274	2.344018
26	6	0.194430	-0.325388	3.300780
27	6	-1.239954	-0.825148	3.231436
28	6	3.381835	0.880275	-0.560254
29	6	4.376404	1.835817	-0.792764
30	1	5.362896	1.523232	-1.121996
31	6	4.081811	3.183317	-0.594024
32	1	4.834409	3.943299	-0.782118
33	6	2.820228	3.533541	-0.114037
34	1	2.536512	4.555780	0.108536
35	6	1.899847	2.517592	0.119427
36	6	0.571828	2.781234	0.795044
37	7	2.157031	1.219432	-0.140575
38	6	-2.605333	0.820709	1.982309
39	1	-1.900692	1.558707	2.369929
40	1	-3.487871	0.795509	2.639206
41	6	-2.993767	1.240832	0.577055
42	6	-4.110682	2.026694	0.291730
43	1	-4.781768	2.332695	1.088371
44	6	-4.341698	2.420586	-1.029575
45	1	-5.204700	3.034627	-1.269625
46	6	-3.455401	2.026912	-2.031439
47	1	-3.579170	2.310873	-3.070218
48	6	-2.360643	1.246233	-1.666882
49	6	-1.289901	0.805324	-2.654593
50	7	-2.158233	0.853502	-0.399738
51	8	-0.244930	0.257328	-2.067649
52	8	-1.450616	0.963589	-3.850450
53	8	0.214675	3.917737	1.055284
54	8	-0.060403	1.673848	1.087598
55	1	-1.218415	-1.914183	3.336916
56	1	-1.795239	-0.428656	4.095188
57	1	0.637308	-0.656397	4.247898
58	1	0.261266	0.763307	3.225677
59	1	2.662028	-0.996110	3.365198
60	1	2.604247	0.335231	2.188793
61	1	4.186879	-1.502903	1.537347
62	1	2.875354	-2.671449	1.679974
63	1	-0.352183	-3.674739	-2.876409
64	1	-0.921739	-1.986463	-2.809948

65	1	-1.356092	-4.237989	-0.754260
66	1	-2.638102	-3.435919	-1.708881

E(RB3LYP) = -1718.207837 Hartrees
Corrección de punto cero = 0.542356 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.632624 Hartrees
Suma de las energías libres y térmicas = -1717.727506 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	0.026499	-0.109946	0.078391
2	7	2.591038	-1.402004	-0.313935
3	7	-1.870781	-0.485450	1.960099
4	8	0.862332	-1.387339	2.010376
5	8	-1.887179	-1.808360	-0.443970
6	8	0.348592	-2.644948	-1.408888
7	6	-2.769469	-1.654427	1.735088
8	1	-2.958359	-2.191934	2.674871
9	1	-3.732091	-1.278400	1.379436
10	6	-2.243399	-2.617765	0.676583
11	1	-1.375104	-3.197398	1.017273
12	1	-3.034859	-3.325393	0.398751
13	6	-1.973603	-2.397259	-1.745206
14	6	-0.768252	-3.286854	-2.016718
15	6	1.605485	-2.941047	-2.008545
16	1	1.759885	-2.291035	-2.879624
17	1	1.638020	-3.984298	-2.349613
18	6	2.652166	-2.749212	-0.928302
19	1	2.460632	-3.494322	-0.152831
20	1	3.657264	-2.953489	-1.330146
21	6	3.101875	-1.453357	1.075356
22	1	3.296237	-0.433012	1.410108
23	1	4.053621	-2.007332	1.136428
24	6	3.368934	-0.461369	-1.156926
25	1	2.983886	-0.543785	-2.179803
26	1	4.432718	-0.748968	-1.187831
27	6	2.116899	-2.094818	2.047490
28	1	1.933003	-3.154234	1.829335
29	1	2.533674	-2.025972	3.059607
30	6	0.000092	-1.665397	3.135139
31	1	0.592976	-1.627556	4.056831
32	1	-0.403008	-2.681617	3.033735
33	6	-1.087285	-0.602272	3.211895
34	1	-0.610237	0.363668	3.385972
35	1	-1.731582	-0.834060	4.075519
36	6	3.244506	0.972702	-0.700818
37	6	4.241332	1.921828	-0.935393
38	1	5.143613	1.644403	-1.471784
39	6	4.058748	3.223017	-0.464111
40	1	4.816064	3.980011	-0.645183
41	6	2.912537	3.527731	0.269307
42	1	2.729989	4.506350	0.698221
43	6	1.974782	2.519786	0.471831
44	6	0.739975	2.710137	1.331102
45	7	2.124867	1.281271	-0.033451
46	6	-2.667293	0.779152	1.955760
47	1	-2.045827	1.557967	2.402972

48	1	-3.578941	0.670871	2.559798
49	6	-3.006430	1.230993	0.548593
50	6	-4.188741	1.895039	0.216889
51	1	-4.952475	2.062170	0.970198
52	6	-4.365870	2.348090	-1.094064
53	1	-5.276320	2.873255	-1.367659
54	6	-3.373955	2.114273	-2.046176
55	1	-3.463152	2.433289	-3.078329
56	6	-2.227183	1.433442	-1.642804
57	6	-1.092592	1.075104	-2.598022
58	7	-2.060422	1.017391	-0.378157
59	8	-0.098995	0.445084	-2.007852
60	8	-1.182959	1.348825	-3.780860
61	8	0.515998	3.781899	1.867111
62	8	0.023529	1.618777	1.425553
63	1	-0.886872	-4.293099	-1.589163
64	1	-0.629566	-3.388285	-3.100433
65	1	-1.983818	-1.553829	-2.436331
66	1	-2.913802	-2.952881	-1.847423

E(RB3LYP) = -1718.2117647 Hartrees
Corrección de punto cero = 0.541756 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.636873 Hartrees
Suma de las energías libres y térmicas = -1717.732202 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λλ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	71	0.166327	-0.066187	0.014007
2	7	1.958866	-1.868893	-0.896140
3	7	-1.622121	-0.295442	1.963853
4	8	0.852278	-1.684765	1.671951
5	8	-3.537616	-1.024669	-0.368096
6	8	-0.940600	-2.200930	-0.885213
7	6	-2.635497	-1.393794	1.919444
8	6	-3.845180	-1.198561	1.000516
9	6	-3.355058	-2.191874	-1.154674
10	6	-2.014940	-2.112891	-1.859099
11	6	-0.042696	-3.312091	-1.051905
12	6	1.234803	-2.852852	-1.738970
13	6	2.617581	-2.554614	0.258872
14	6	2.926199	-1.096840	-1.718811
15	1	2.394240	-0.759962	-2.615868
16	1	3.770299	-1.724252	-2.041703
17	6	2.264258	-1.983826	1.637764
18	6	0.198761	-1.726839	2.966146
19	6	-0.717816	-0.516146	3.127721
20	6	3.417414	0.125142	-0.977753
21	6	4.687578	0.677493	-1.143516
22	1	5.406173	0.209446	-1.809137
23	6	5.010908	1.842584	-0.442008
24	1	5.991545	2.293876	-0.560944
25	6	4.072420	2.409678	0.419970
26	1	4.272073	3.301903	1.002375
27	6	2.830163	1.791787	0.537956
28	6	1.741942	2.287633	1.477035
29	7	2.516210	0.683898	-0.155799
30	6	-2.253596	1.054563	2.070153

31	1	-1.525831	1.713259	2.551934
32	1	-3.148511	1.027950	2.707126
33	6	-2.569390	1.665388	0.716255
34	6	-3.609507	2.571774	0.506583
35	1	-4.282657	2.832268	1.317762
36	6	-3.764431	3.140393	-0.760575
37	1	-4.566605	3.849945	-0.941130
38	6	-2.891113	2.788218	-1.790075
39	1	-2.970559	3.193409	-2.792252
40	6	-1.880544	1.874575	-1.505576
41	6	-0.876489	1.393211	-2.548616
42	7	-1.735055	1.342030	-0.281057
43	8	0.008083	0.544036	-2.063234
44	8	-0.958827	1.779501	-3.699210
45	8	1.944896	3.249205	2.196520
46	8	0.651748	1.562651	1.412327
47	1	1.868376	-3.722009	-1.977551
48	1	0.971426	-2.364078	-2.681247
49	1	-0.526312	-4.101959	-1.635528
50	1	0.155736	-3.710064	-0.053070
51	1	-1.917494	-2.926285	-2.585552
52	1	-1.910911	-1.163943	-2.388135
53	1	-3.407678	-3.102033	-0.541961
54	1	-4.151475	-2.243635	-1.910568
55	1	-4.504427	-2.066513	1.148950
56	1	-4.418332	-0.314894	1.293765
57	1	-2.117582	-2.314026	1.632926
58	1	-3.041524	-1.547579	2.934092
59	1	-0.098231	0.376300	3.224575
60	1	-1.291058	-0.646381	4.060172
61	1	0.951926	-1.696677	3.759652
62	1	-0.334684	-2.680632	3.034704
63	1	2.498105	-2.733929	2.401122
64	1	2.821402	-1.069407	1.863476
65	1	3.708636	-2.524082	0.148292
66	1	2.335061	-3.610770	0.241831

E(RB3LYP) = -1718.2085561 Hartrees
Corrección de punto cero = 0.541923 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.633735 Hartrees
Suma de las energías libres y térmicas = -1717.728238 Hartrees

[Lu(dpa15c5)]$^{+}$ (vacío) Λ(λδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	71	0	-0.033390	0.076630	0.020379
2	7	0	-2.491937	1.538499	-0.494775
3	7	0	1.721826	0.098029	2.063656
4	8	0	-0.984859	1.085631	2.009493
5	8	0	1.995061	1.870488	-0.053740
6	8	0	-0.136361	2.965462	-1.029560
7	6	0	2.603766	1.284047	2.148136
8	6	0	3.133276	1.711648	0.790800
9	6	0	2.174961	2.694218	-1.216886
10	6	0	1.058628	3.715003	-1.186974
11	6	0	-1.303010	3.748030	-0.861783
12	6	0	-2.476983	2.848646	-1.197660
13	6	0	-3.066710	1.634800	0.870754

14	1	0	-3.476311	0.657891	1.136016
15	1	0	-3.901258	2.354688	0.900424
16	6	0	-3.305000	0.628526	-1.349703
17	1	0	-2.846022	0.636916	-2.344639
18	1	0	-4.334931	1.003744	-1.459821
19	6	0	-2.079792	2.023455	1.970254
20	1	0	-1.675107	3.034011	1.849376
21	1	0	-2.610733	1.984473	2.929449
22	6	0	-0.250994	1.100530	3.255034
23	1	0	-0.946947	0.891940	4.076607
24	1	0	0.155582	2.108282	3.406223
25	6	0	0.828496	0.018939	3.246971
26	1	0	0.345660	-0.958405	3.218368
27	1	0	1.389552	0.100547	4.192111
28	6	0	-3.329633	-0.793151	-0.856262
29	6	0	-4.429653	-1.629648	-1.056914
30	1	0	-5.314181	-1.252368	-1.560683
31	6	0	-4.370081	-2.947280	-0.601003
32	1	0	-5.209998	-3.618308	-0.754542
33	6	0	-3.230271	-3.377929	0.075000
34	1	0	-3.128382	-4.376964	0.483049
35	6	0	-2.184358	-2.475434	0.246142
36	6	0	-0.940082	-2.823826	1.032382
37	7	0	-2.222345	-1.217020	-0.230321
38	6	0	2.529848	-1.146729	1.908029
39	1	0	1.909372	-1.985045	2.231645
40	1	0	3.423562	-1.111735	2.547966
41	6	0	2.922640	-1.419994	0.466642
42	6	0	4.076646	-2.122890	0.112081
43	1	0	4.772901	-2.453567	0.876764
44	6	0	4.312954	-2.398419	-1.237585
45	1	0	5.202191	-2.948939	-1.530485
46	6	0	3.404838	-1.961038	-2.202638
47	1	0	3.539622	-2.144176	-3.262518
48	6	0	2.279203	-1.262732	-1.773239
49	6	0	1.212647	-0.733320	-2.727993
50	7	0	2.059285	-1.007087	-0.472766
51	8	0	0.198397	-0.169656	-2.106085
52	8	0	1.363010	-0.846821	-3.929971
53	8	0	-0.820781	-3.916964	1.559902
54	8	0	-0.088151	-1.834316	1.082911
55	1	0	1.192321	4.405336	-0.339967
56	1	0	1.033299	4.300034	-2.117564
57	1	0	2.109806	2.067579	-2.111751
58	1	0	3.153055	3.185698	-1.196267
59	1	0	-3.422378	3.390325	-1.032935
60	1	0	-2.403840	2.635778	-2.266620
61	1	0	-1.343748	4.169267	0.153376
62	1	0	-1.309942	4.594437	-1.563851
63	1	0	3.659434	2.668860	0.899510
64	1	0	3.831949	0.985342	0.360170
65	1	0	3.443313	1.103474	2.837593
66	1	0	2.026492	2.119927	2.550411

E(RB3LYP) = -1718.210919 Hartrees
Corrección de punto cero = 0.542189 Hartrees
Suma de las entalpías electrónicas y térmicas = -1717.635670 Hartrees
Suma de las energías libres y térmicas = -1717.731497 Hartrees

[La(dpa18c6)]$^{+}$ (vacío) Δ(λλλ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.718778	1.300881	0.527898
2	7	-2.670103	0.632213	1.336478
3	8	-2.132280	1.726629	-1.238381
4	6	-3.473489	1.279210	-0.976470
5	6	-2.460536	1.357780	2.614078
6	6	-1.722732	2.680718	2.423699
7	8	-0.375601	2.505580	1.949654
8	6	0.588479	2.290613	2.996227
9	6	1.971589	2.520026	2.424494
10	8	2.132234	1.726672	1.238379
11	8	0.375536	2.505600	-1.949646
12	6	-0.588538	2.290622	-2.996222
13	6	-1.971653	2.520000	-2.424487
14	7	2.670078	0.632277	-1.336483
15	6	2.460496	1.357849	-2.614078
16	6	1.722664	2.680770	-2.423690
17	6	3.473453	1.279280	0.976469
18	6	3.718742	1.300957	-0.527900
19	6	-3.009177	-0.785194	1.618669
20	6	3.009175	-0.785122	-1.618686
21	6	2.872138	-1.685560	-0.409807
22	6	-2.872111	-1.685625	0.409788
23	6	1.649635	-2.205395	1.501763
24	6	2.452743	-3.310819	1.778163
25	6	3.511141	-3.591451	0.915901
26	6	3.734440	-2.761558	-0.184520
27	6	-3.734385	-2.761643	0.184493
28	6	-3.511051	-3.591535	-0.915922
29	6	-2.452645	-3.310884	-1.778169
30	6	-1.649570	-2.205438	-1.501765
31	57	-0.000010	0.504938	0.000000
32	1	-3.773063	2.348808	0.831531
33	1	-4.709307	0.864078	0.730247
34	1	-4.189401	1.961745	-1.449610
35	1	-3.605803	0.284825	-1.412817
36	1	3.605786	0.284897	1.412815
37	1	4.189350	1.961829	1.449610
38	1	3.773013	2.348886	-0.831529
39	1	4.709278	0.864170	-0.730249
40	1	-4.026441	-0.870123	2.032522
41	1	-2.303911	-1.139330	2.376744
42	1	4.026438	-0.870029	-2.032547
43	1	2.303911	-1.139268	-2.376758
44	1	2.234552	-3.907638	2.656239
45	1	4.164970	-4.438581	1.102081
46	1	4.561869	-2.945936	-0.862681
47	1	-4.561819	-2.946040	0.862643
48	1	-4.164857	-4.438681	-1.102109
49	1	-2.234423	-3.907707	-2.656236
50	7	-1.846915	-1.427980	-0.421024
51	7	1.846944	-1.427939	0.421015
52	6	0.512784	-1.798285	2.432620
53	8	-0.035557	-0.654072	2.131200
54	8	0.206078	-2.531675	3.362632
55	6	-0.512710	-1.798306	-2.432601

56	8	0.035552	-0.654046	-2.131215
57	8	-0.205928	-2.531720	-3.362569
58	1	0.492411	1.269694	3.379367
59	1	0.418786	3.010326	3.807651
60	1	2.709551	2.228204	3.181049
61	1	2.124045	3.575426	2.166164
62	1	-0.492449	1.269709	-3.379372
63	1	-0.418861	3.010346	-3.807639
64	1	-2.124130	3.575394	-2.166146
65	1	-2.709609	2.228171	-3.181044
66	1	2.207914	3.322239	-1.683781
67	1	1.704873	3.229291	-3.373550
68	1	3.418435	1.558450	-3.123137
69	1	1.868422	0.710294	-3.264009
70	1	-1.704952	3.229232	3.373564
71	1	-2.207997	3.322182	1.683796
72	1	-3.418480	1.558358	3.123138
73	1	-1.868449	0.710232	3.264005

E(RB3LYP) = -1863.6755323 Hartree
Corrección de punto cero = 0.604931
Suma de las entalpías electrónicas y térmicas = -1863.034340
Suma de las energías libres y térmicas = -1863.135661

[La(dpa18c6)]$^{+}$ (vacío) Δ(δδδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.706697	-0.954499	-0.505393
2	7	2.915504	-0.617259	0.700060
3	8	1.767143	-1.778386	-1.653519
4	6	3.117269	-2.111219	-1.300175
5	6	3.185372	-1.590431	1.787027
6	6	1.961460	-1.925363	2.623001
7	8	0.976426	-2.512340	1.737155
8	6	-0.036971	-3.289446	2.392025
9	6	-1.212329	-2.425411	2.817029
10	8	-1.762445	-1.780815	1.655457
11	8	-0.969817	-2.515541	-1.737102
12	6	0.045463	-3.290031	-2.392173
13	6	1.219201	-2.423240	-2.815980
14	7	-2.913743	-0.625369	-0.699968
15	6	-3.181225	-1.599576	-1.786581
16	6	-1.956628	-1.931329	-2.622788
17	6	-3.111000	-2.118831	1.301034
18	6	-3.703978	-0.964354	0.505645
19	6	3.207523	0.769414	1.149311
20	6	-3.209327	0.760390	-1.149727
21	6	-2.775564	1.792315	-0.126617
22	6	2.770879	1.799861	0.125929
23	6	-1.258519	2.331860	1.558608
24	6	-1.895012	3.545004	1.815005
25	6	-3.015623	3.875477	1.053949
26	6	-3.476404	2.981920	0.084448
27	6	3.468326	2.991415	-0.085393
28	6	3.004910	3.883524	-1.054974
29	6	1.885112	3.549820	-1.815823
30	6	1.252132	2.334879	-1.559229
31	57	0.000787	-0.506578	0.000035

32	1	0.390262	-3.813307	3.256652
33	1	-0.363776	-4.036942	1.661939
34	1	-0.896221	-1.635800	3.505836
35	1	-1.973096	-3.041620	3.309298
36	1	-0.380310	-3.814027	-3.257433
37	1	0.373552	-4.037472	-1.662609
38	1	1.981553	-3.037624	-3.308069
39	1	0.901847	-1.633880	-3.504518
40	1	4.281418	0.894064	1.363355
41	1	2.653555	0.939605	2.077919
42	1	-4.283515	0.882141	-1.363973
43	1	-2.655685	0.931723	-2.078330
44	1	-1.506841	4.184926	2.598990
45	1	-3.541466	4.810260	1.225447
46	1	-4.365836	3.201702	-0.497858
47	1	4.357188	3.213834	0.496783
48	1	3.528094	4.819763	-1.226666
49	1	1.494987	4.188595	-2.599773
50	7	1.674504	1.502996	-0.590968
51	7	-1.678367	1.498680	0.590360
52	6	-0.060984	1.860008	2.378535
53	8	0.321594	0.641441	2.107135
54	8	0.442184	2.616939	3.197380
55	6	0.055748	1.859493	-2.378796
56	8	-0.322709	0.639565	-2.107697
57	8	-0.450318	2.615121	-3.197058
58	1	4.751068	-1.196761	-0.247036
59	1	3.713853	-2.248189	-2.210098
60	1	3.129100	-3.054820	-0.738800
61	1	-4.747584	-1.209945	0.247351
62	1	-3.728221	-0.088904	1.157127
63	1	-3.707765	-2.257893	2.210533
64	1	-3.118935	-3.062524	0.739737
65	1	-1.539990	-1.043204	-3.106678
66	1	-2.234441	-2.672493	-3.382746
67	1	-3.540100	-2.530540	-1.338825
68	1	-3.979880	-1.237292	-2.451815
69	1	2.241083	-2.665679	3.383126
70	1	1.542325	-1.038286	3.106648
71	1	3.982812	-1.225765	2.452409
72	1	3.546950	-2.520522	1.339641
73	1	3.728232	-0.079290	-1.157292

E(RB3LYP) = -1863.6764369 Hartree
Corrección de punto cero = 0.604148
Suma de las entalpías electrónicas y térmicas = -1863.035919
Suma de las energías libres y térmicas = -1863.137845

[La(dpa18c6)]$^{+}$ (vacío) Δ(δλλ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.729073	-0.952354	0.185131
2	7	-2.814386	-0.480437	-0.880990
3	8	-1.896317	-1.891639	1.459987
4	6	-3.238742	-2.128963	1.024069
5	6	-2.896996	-1.265297	-2.134260
6	6	-2.208499	-2.626333	-2.080623
7	8	-0.808407	-2.533996	-1.756990

8	6	0.068783	-2.492148	-2.897764
9	6	1.462070	-2.849123	-2.432257
10	8	1.897212	-1.890916	-1.459863
11	8	0.809569	-2.533480	1.757101
12	6	-0.067599	-2.491949	2.897904
13	6	-1.460743	-2.849570	2.432458
14	7	2.814683	-0.479092	0.880943
15	6	2.897627	-1.263858	2.134248
16	6	2.209717	-2.625195	2.080680
17	6	3.239767	-2.127566	-1.023982
18	6	3.729569	-0.950663	-0.185153
19	6	-3.133010	0.942328	-1.188850
20	6	3.132680	0.943825	1.188724
21	6	2.755592	1.869741	0.051768
22	6	-2.756427	1.868445	-0.051894
23	6	1.275258	2.291860	-1.694809
24	6	1.933954	3.470779	-2.038399
25	6	3.053917	3.841715	-1.295419
26	6	3.482469	3.024828	-0.247486
27	6	-3.483910	3.023156	0.247351
28	6	-3.055819	3.840242	1.295317
29	6	-1.935698	3.469863	2.038335
30	6	-1.276373	2.291295	1.694739
31	57	0.000131	-0.486882	-0.000009
32	1	-4.201252	1.063620	-1.428629
33	1	-2.557372	1.225490	-2.074737
34	1	4.200882	1.065617	1.428430
35	1	2.556967	1.226754	2.074634
36	1	1.562509	4.053571	-2.873379
37	1	3.600229	4.748741	-1.537506
38	1	4.365824	3.277640	0.330762
39	1	-4.367369	3.275521	-0.330931
40	1	-3.602605	4.746983	1.537398
41	1	-1.564592	4.052817	2.873352
42	7	-1.668087	1.528391	0.658100
43	7	1.667408	1.529135	-0.658203
44	6	0.074666	1.782429	-2.482931
45	8	-0.300708	0.577401	-2.155614
46	8	-0.445301	2.503791	-3.324593
47	6	-0.075564	1.782467	2.482922
48	8	0.300537	0.577694	2.155503
49	8	0.443868	2.504009	3.324757
50	1	-4.717652	-1.215425	-0.227702
51	1	-3.895191	-2.213618	1.901336
52	1	-3.283527	-3.087853	0.494263
53	1	4.718278	-1.213245	0.227683
54	1	3.882797	-0.113277	-0.869376
55	1	3.896222	-2.211969	-1.901268
56	1	3.285037	-3.086397	-0.494107
57	1	-1.471729	-3.854479	1.987771
58	1	-2.142318	-2.836370	3.293903
59	1	-0.045457	-1.493001	3.347551
60	1	0.253065	-3.237612	3.636314
61	1	-3.882703	-0.114987	0.869287
62	1	2.143652	-2.835699	-3.293692
63	1	1.473492	-3.853988	-1.987482
64	1	-0.251529	-3.237998	-3.636138
65	1	0.046220	-1.493237	-3.347472
66	1	-3.947467	-1.423488	-2.435223
67	1	-2.412899	-0.670090	-2.911508

68	1	-2.325291	-3.116426	-3.054773
69	1	-2.645973	-3.289814	-1.334172
70	1	2.647447	-3.288509	1.334229
71	1	2.326762	-3.115209	3.054839
72	1	2.413279	-0.668823	2.911470
73	1	3.948167	-1.421585	2.435215

E(RB3LYP) = -1863.680023 Hartree
Corrección de punto cero = 0.605022
Suma de las entalpías electrónicas y térmicas = -1863.038884
Suma de las energías libres y térmicas = -1863.139528

[La(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.748915	1.192192	-0.375286
2	7	2.730790	0.532352	-1.231384
3	8	2.058758	1.958084	1.145141
4	6	3.347431	1.323187	1.088590
5	6	2.573044	1.241754	-2.522787
6	6	1.879752	2.590966	-2.398442
7	8	0.564444	2.394199	-1.857863
8	6	-0.455942	3.289124	-2.307810
9	6	-1.750583	2.512651	-2.429626
10	8	-2.058739	1.958024	-1.145214
11	8	-0.564409	2.394184	1.857892
12	6	0.455935	3.289277	2.307603
13	6	1.750639	2.512918	2.429470
14	7	-2.730776	0.532401	1.231404
15	6	-2.573001	1.241755	2.522831
16	6	-1.879689	2.590959	2.398532
17	6	-3.347445	1.323204	-1.088572
18	6	-3.748867	1.192319	0.375329
19	6	3.067897	-0.888130	-1.497563
20	6	-3.067953	-0.888073	1.497543
21	6	-2.890940	-1.774589	0.284760
22	6	2.890889	-1.774644	-0.284777
23	6	-1.602098	-2.260717	-1.591838
24	6	-2.383569	-3.371434	-1.905317
25	6	-3.468267	-3.670000	-1.082655
26	6	-3.735407	-2.855258	0.019583
27	6	3.735354	-2.855316	-0.019603
28	6	3.468232	-3.670042	1.082650
29	6	2.383556	-3.371455	1.905333
30	6	1.602081	-2.260739	1.591854
31	57	-0.000008	0.436273	0.000011
32	1	3.929784	2.200407	-0.757328
33	1	4.710148	0.660248	-0.427825
34	1	4.085499	1.953767	1.602123
35	1	3.300848	0.357620	1.602148
36	1	1.956605	0.608270	-3.163497
37	1	3.546115	1.397019	-3.019293
38	1	1.799959	3.024283	-3.402878
39	1	2.427891	3.301930	-1.767738
40	1	-0.195687	3.699267	-3.290966
41	1	-0.563520	4.121662	-1.599892
42	1	-1.646204	1.707615	-3.168381
43	1	-2.555942	3.190443	-2.744031

44	1	0.195716	3.699575	3.290704
45	1	0.563393	4.121697	1.599529
46	1	2.555971	3.190818	2.743710
47	1	1.646359	1.708007	3.168377
48	1	-1.956562	0.608238	3.163509
49	1	-3.546061	1.397021	3.019356
50	1	-2.427838	3.301976	1.767893
51	1	-1.799844	3.024213	3.402991
52	1	-3.300944	0.357606	-1.602080
53	1	-4.085499	1.953801	-1.602106
54	1	-3.929590	2.200574	0.757333
55	1	-4.710164	0.660494	0.427948
56	1	4.095581	-0.982835	-1.882695
57	1	2.383327	-1.242479	-2.275031
58	1	-4.095655	-0.982739	1.882640
59	1	-2.383427	-1.242463	2.275030
60	1	-2.128982	-3.958788	-2.780003
61	1	-4.107990	-4.520504	-1.299942
62	1	-4.581994	-3.055634	0.668962
63	1	4.581927	-3.055703	-0.668996
64	1	4.107955	-4.520546	1.299937
65	1	2.128987	-3.958787	2.780038
66	7	1.843909	-1.495755	0.510978
67	7	-1.843946	-1.495716	-0.510980
68	6	-0.431447	-1.833156	-2.469914
69	8	0.071162	-0.674690	-2.147547
70	8	-0.057231	-2.569298	-3.372806
71	6	0.431464	-1.833164	2.469970
72	8	-0.071247	-0.674764	2.147525
73	8	0.057338	-2.569257	3.372937

E(RB3LYP) = -1863.67932 Hartree
Corrección de punto cero = 0.604071
Suma de las entalpías electrónicas y térmicas = -1863.038645
Suma de las energías libres y térmicas = -1863.141780

[La(dpa18c6)]$^{+}$ (vacío) Δ(λλδ)(λλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.701589	-0.952139	0.671889
2	7	-2.931133	-0.645274	-0.568885
3	8	-1.800252	-2.268874	1.344311
4	6	-2.810973	-1.370268	1.843345
5	6	-3.208803	-1.674740	-1.600603
6	6	-2.144988	-1.796564	-2.675105
7	8	-0.933224	-2.280651	-2.065611
8	6	0.069395	-2.592072	-3.038473
9	6	1.252224	-3.185304	-2.299732
10	8	1.803773	-2.266759	-1.343832
11	8	0.936740	-2.278797	2.066084
12	6	-0.065425	-2.591451	3.039005
13	6	-1.247361	-3.186517	2.300326
14	7	2.932149	-0.640760	0.568931
15	6	3.211368	-1.669589	1.600873
16	6	2.147773	-1.792730	2.675445
17	6	2.812922	-1.366462	-1.843077
18	6	3.703008	-0.946813	-0.671785
19	6	-3.234524	0.717107	-1.072374

20	6	3.233603	0.722170	1.072068
21	6	2.755196	1.776777	0.096374
22	6	-2.757769	1.772569	-0.096798
23	6	1.174618	2.317472	-1.526835
24	6	1.757877	3.560978	-1.758671
25	6	2.891016	3.903639	-1.020173
26	6	3.409753	2.996201	-0.094007
27	6	-3.414469	2.990815	0.093732
28	6	-2.897336	3.899061	1.020002
29	6	-1.763625	3.558274	1.758487
30	6	-1.178142	2.315853	1.526444
31	57	0.000513	-0.605009	-0.000083
32	1	-4.425645	-1.747613	0.465141
33	1	-4.279803	-0.077367	0.987306
34	1	-3.416064	-1.883220	2.601091
35	1	-2.330338	-0.503729	2.310518
36	1	2.330758	-0.500723	-2.310168
37	1	3.418743	-1.878431	-2.600900
38	1	4.428192	-1.741225	-0.464902
39	1	4.279962	-0.071309	-0.987459
40	1	-4.312967	0.839836	-1.261966
41	1	-2.707799	0.860042	-2.021035
42	1	4.311886	0.846512	1.261538
43	1	2.706791	0.864536	2.020769
44	1	1.324518	4.214738	-2.506894
45	1	3.380120	4.860878	-1.175689
46	1	4.306629	3.228518	0.471725
47	1	-4.311759	3.221595	-0.471971
48	1	-3.388129	4.855417	1.175629
49	1	-1.331492	4.212650	2.506883
50	7	-1.653467	1.464142	0.600838
51	7	1.651511	1.466464	-0.601386
52	6	-0.024163	1.812889	-2.320251
53	8	-0.297686	0.553658	-2.107256
54	8	-0.627741	2.575689	-3.062579
55	6	0.021401	1.813205	2.319959
56	8	0.297045	0.554467	2.106848
57	8	0.623475	2.576869	3.062616
58	1	2.489912	-2.526955	3.417473
59	1	1.934389	-0.845319	3.179607
60	1	4.182911	-1.483098	2.088426
61	1	3.278939	-2.635536	1.094296
62	1	-2.485982	-2.531477	-3.416967
63	1	-1.933033	-0.848957	-3.179488
64	1	-3.275041	-2.640678	-1.093840
65	1	-4.180582	-1.489768	-2.088273
66	1	0.343777	-1.682206	-3.588227
67	1	-0.321450	-3.330784	-3.752683
68	1	2.027444	-3.501145	-3.008162
69	1	0.930849	-4.057531	-1.722689
70	1	-0.341071	-1.681888	3.588635
71	1	0.326465	-3.329482	3.753352
72	1	-0.924628	-4.058307	1.723383
73	1	-2.022147	-3.503447	3.008736

E(RB3LYP) = -1863.6702584 Hartree
Corrección de punto cero = 0.604744
Suma de las entalpías electrónicas y térmicas = -1863.029347
Suma de las energías libres y térmicas = -1863.129625

[La(dpa18c6)]$^{+}$ (vacío) Δ(δδλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.729588	0.906206	-0.129335
2	7	2.687233	0.896205	0.920539
3	8	2.656349	-0.970858	-1.216851
4	6	3.929133	-0.401838	-0.888612
5	6	3.087805	0.208510	2.168473
6	6	3.041142	-1.319060	2.135700
7	8	1.730877	-1.761818	1.751947
8	6	1.173109	-2.881473	2.453029
9	6	-0.296574	-2.583712	2.709702
10	8	-0.985850	-2.269658	1.492232
11	8	0.491374	-2.647191	-1.524123
12	6	1.812542	-3.155495	-1.754226
13	6	2.712290	-2.017347	-2.198801
14	7	-2.169746	-1.735792	-1.069717
15	6	-1.754360	-2.329314	-2.359032
16	6	-0.567316	-3.277281	-2.267104
17	6	-1.672300	-3.338773	0.833361
18	6	-2.710021	-2.723141	-0.105200
19	6	2.325580	2.306480	1.245328
20	6	-3.177597	-0.676124	-1.348463
21	6	-3.382170	0.252506	-0.170340
22	6	1.617645	2.992784	0.095439
23	6	-2.386485	1.381622	1.605475
24	6	-3.590131	1.987108	1.962934
25	6	-4.728007	1.688061	1.215773
26	6	-4.629534	0.796578	0.145374
27	6	1.754572	4.357090	-0.169954
28	6	1.036918	4.913833	-1.231152
29	6	0.227811	4.094817	-2.017881
30	6	0.160868	2.738249	-1.705740
31	57	0.188495	-0.318728	-0.033060
32	1	2.387627	0.532474	2.941568
33	1	4.102943	0.509303	2.481394
34	1	3.267293	-1.673939	3.148409
35	1	3.780777	-1.761249	1.460948
36	1	1.684376	-3.023568	3.412811
37	1	1.308234	-3.792800	1.854763
38	1	-0.384234	-1.691431	3.334315
39	1	-0.779297	-3.429998	3.213869
40	1	1.795671	-3.936953	-2.522227
41	1	2.183092	-3.595751	-0.820781
42	1	3.738963	-2.388840	-2.302298
43	1	2.382809	-1.611242	-3.162377
44	1	-1.475529	-1.495475	-3.006475
45	1	-2.585308	-2.879878	-2.833876
46	1	-0.822382	-4.234033	-1.793347
47	1	-0.225710	-3.490763	-3.287211
48	1	3.216924	2.885427	1.534711
49	1	1.643676	2.276985	2.100312
50	1	-4.140644	-1.116660	-1.650294
51	1	-2.801958	-0.086329	-2.190746
52	1	-3.604396	2.659220	2.813178
53	1	-5.686882	2.130516	1.469947
54	1	-5.504181	0.529909	-0.439868
55	1	2.408145	4.969758	0.443250

56	1	1.122483	5.974713	-1.447974
57	1	-0.341437	4.467065	-2.861845
58	7	0.824935	2.215035	-0.659596
59	7	-2.288139	0.556623	0.547659
60	6	-1.110124	1.598436	2.412505
61	8	-0.139486	0.788669	2.092715
62	8	-1.081803	2.472257	3.268889
63	6	-0.662484	1.754682	-2.532314
64	8	-0.463038	0.505476	-2.214414
65	8	-1.427337	2.180839	-3.387078
66	1	3.436794	1.664298	-0.858467
67	1	4.706356	1.213060	0.282962
68	1	4.483380	-0.174808	-1.808660
69	1	4.518557	-1.133975	-0.322700
70	1	-3.246814	-3.534511	-0.623452
71	1	-3.438786	-2.206918	0.525071
72	1	-2.199794	-3.949569	1.577926
73	1	-0.955007	-3.983239	0.313227

E(RB3LYP) = -1863.6713684 Hartree
Corrección de punto cero = 0.603610
Suma de las entalpías electrónicas y térmicas = -1863.030943
Suma de las energías libres y térmicas = -1863.135351

[La(dpa18c6)]$^{+}$ (vacío) Δ(λδδ)(λδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.808273	1.100982	0.357927
2	7	2.932030	0.735349	-0.790855
3	8	1.899953	1.841029	1.619783
4	6	3.119825	1.088201	1.719958
5	6	3.112235	1.690342	-1.916286
6	6	1.867473	1.897530	-2.760723
7	8	0.853538	2.481087	-1.907155
8	6	-0.197736	3.169521	-2.600784
9	6	-1.377708	2.262039	-2.888583
10	8	-1.900114	1.841074	-1.619642
11	8	-0.853738	2.480830	1.907359
12	6	0.197486	3.169245	2.601087
13	6	1.377518	2.261804	2.888774
14	7	-2.932112	0.735043	0.790860
15	6	-3.112391	1.689954	1.916347
16	6	-1.867669	1.897145	2.760842
17	6	-3.119894	1.088112	-1.719919
18	6	-3.808376	1.100688	-0.357904
19	6	3.183532	-0.652343	-1.256588
20	6	-3.183527	-0.652696	1.256500
21	6	-2.777762	-1.693677	0.234810
22	6	2.777891	-1.693414	-0.234943
23	6	-1.274055	-2.277671	-1.445902
24	6	-1.907114	-3.499699	-1.662164
25	6	-3.026024	-3.807998	-0.888573
26	6	-3.480869	-2.888129	0.058297
27	6	3.481151	-2.887780	-0.058467
28	6	3.026427	-3.807733	0.888381
29	6	1.907483	-3.499597	1.661985
30	6	1.274265	-2.277645	1.445759
31	57	-0.000038	0.632205	0.000010

32	1	4.183699	2.114244	0.196009
33	1	4.688059	0.443517	0.410137
34	1	3.785734	1.573199	2.446231
35	1	2.894567	0.080089	2.078129
36	1	0.185790	3.601559	-3.532580
37	1	-0.514286	3.986580	-1.944718
38	1	-1.080276	1.385599	-3.477455
39	1	-2.147925	2.822462	-3.435936
40	1	-0.186074	3.601131	3.532939
41	1	0.513987	3.986413	1.945133
42	1	2.147697	2.822214	3.436196
43	1	1.080145	1.385273	3.477540
44	1	-2.894506	0.080057	-2.078171
45	1	-3.785842	1.573095	-2.446167
46	1	-4.183925	2.113891	-0.195895
47	1	-4.688085	0.443125	-0.410195
48	1	4.245400	-0.785279	-1.519201
49	1	2.589287	-0.818028	-2.160668
50	1	-4.245395	-0.785730	1.519061
51	1	-2.589306	-0.818392	2.160594
52	1	-1.520761	-4.162952	-2.427541
53	1	-3.552715	-4.747033	-1.031738
54	1	-4.364938	-3.092788	0.653999
55	1	4.365243	-3.092308	-0.654179
56	1	3.553241	-4.746705	1.031519
57	1	1.521221	-4.162915	2.427351
58	7	1.688338	-1.416276	0.498874
59	7	-1.688246	-1.416380	-0.498999
60	6	-0.094752	-1.813697	-2.293375
61	8	0.227999	-0.563175	-2.101698
62	8	0.445619	-2.598411	-3.060910
63	6	0.094913	-1.813850	2.293260
64	8	-0.228027	-0.563373	2.101611
65	8	-0.445321	-2.598653	3.060803
66	1	-2.107434	2.608842	3.560822
67	1	-1.489523	0.967851	3.194787
68	1	-3.938864	1.378642	2.575186
69	1	-3.378494	2.663203	1.497598
70	1	2.107167	2.609307	-3.560653
71	1	1.489369	0.968249	-3.194731
72	1	3.378310	2.663576	-1.497484
73	1	3.938699	1.379108	-2.575171

E(RB3LYP) = -1863.6719561 Hartree
Corrección de punto cero = 0.604750
Suma de las entalpías electrónicas y térmicas = -1863.031050
Suma de las energías libres y térmicas = -1863.131865

[La(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.665153	-1.018264	-0.686083
2	7	2.964645	-0.616697	0.552390
3	8	1.702873	-2.089372	-1.578628
4	6	3.097262	-2.283461	-1.306975
5	6	3.327105	-1.529148	1.662317
6	6	2.243461	-1.670368	2.710831
7	8	1.072209	-2.236245	2.088130

8	6	0.100582	-2.583137	3.076646
9	6	-1.133754	-3.123050	2.398177
10	8	-1.699243	-2.089178	1.581277
11	8	-1.068015	-2.240718	-2.085947
12	6	-0.095840	-2.589343	-3.073299
13	6	1.138897	-3.126079	-2.393005
14	7	-2.963480	-0.622483	-0.553165
15	6	-3.324113	-1.536018	-1.662783
16	6	-2.239428	-1.676888	-2.710263
17	6	-3.092536	-2.288026	1.307348
18	6	-3.663621	-1.024880	0.685250
19	6	3.307825	0.780809	0.916975
20	6	-3.308838	0.774299	-0.918433
21	6	-2.812912	1.780992	0.097110
22	6	2.809750	1.786280	-0.098724
23	6	-1.172363	2.327554	1.654131
24	6	-1.797079	3.532016	1.969987
25	6	-2.982783	3.852783	1.310653
26	6	-3.508488	2.960354	0.374889
27	6	3.502878	2.966976	-0.376958
28	6	2.975124	3.858105	-1.312818
29	6	1.789890	3.534801	-1.971776
30	6	1.167732	2.329126	-1.655509
31	57	0.000675	-0.520721	-0.000029
32	1	4.397237	0.892974	1.042403
33	1	2.832979	0.998996	1.878710
34	1	-4.398379	0.884610	-1.044387
35	1	-2.833948	0.992906	-1.880058
36	1	-1.348045	4.173217	2.719682
37	1	-3.504040	4.779481	1.532455
38	1	-4.443202	3.174022	-0.134198
39	1	4.437293	3.182676	0.131823
40	1	3.494455	4.785796	-1.534985
41	1	1.339375	4.174956	-2.721476
42	7	1.658447	1.491074	-0.724053
43	7	-1.661123	1.488262	0.722749
44	6	0.100242	1.873445	2.355670
45	8	0.465127	0.660244	2.045390
46	8	0.675251	2.633698	3.122829
47	6	-0.104106	1.872081	-2.356523
48	8	-0.465748	0.657870	-2.046361
49	8	-0.681485	2.631125	-3.123099
50	1	4.743958	-1.169448	-0.510015
51	1	3.625385	-2.477181	-2.250105
52	1	3.224216	-3.166432	-0.666973
53	1	-4.741901	-1.179144	0.508670
54	1	-3.565074	-0.215631	1.412039
55	1	-3.621545	-2.483391	2.249637
56	1	-3.215413	-3.171503	0.667244
57	1	-1.966764	-0.718883	-3.162097
58	1	-2.591723	-2.364063	-3.491732
59	1	-3.521033	-2.528576	-1.250741
60	1	-4.253738	-1.206685	-2.153779
61	1	2.597277	-2.356331	3.492684
62	1	1.970020	-0.712270	3.162001
63	1	4.256837	-1.198578	2.152287
64	1	3.524613	-2.521789	1.250780
65	1	0.907868	-4.004254	-1.773863
66	1	1.861208	-3.425052	-3.163340
67	1	0.157949	-1.702751	-3.668969

68	1	-0.503927	-3.361447	-3.741185
69	1	3.563925	-0.209818	-1.413398
70	1	-1.855488	-3.420758	3.169559
71	1	-0.901929	-4.002640	1.781325
72	1	0.509592	-3.353000	3.746551
73	1	-0.153941	-1.695155	3.669909

E(RB3LYP) =-1863.6847146 Hartree
Corrección de punto cero = 0.604536
Suma de las entalpías electrónicas y térmicas = -1863.043840
Suma de las energías libres y térmicas = -1863.145367

[Ce(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.755734	-1.140990	-0.082063
2	7	-2.789313	-0.544456	-1.040232
3	8	-1.969446	-1.934512	1.306659
4	6	-3.234720	-1.253523	1.345525
5	6	-2.741233	-1.316316	-2.303980
6	6	-2.051542	-2.666537	-2.162050
7	8	-0.691569	-2.462252	-1.744089
8	6	0.313129	-3.270548	-2.366101
9	6	1.550703	-2.423700	-2.580655
10	8	1.976926	-1.930466	-1.303656
11	8	0.700844	-2.457831	1.745394
12	6	-0.300833	-3.264192	2.374830
13	6	-1.540249	-2.419164	2.586012
14	7	2.792157	-0.532533	1.039609
15	6	2.747545	-1.304925	2.303145
16	6	2.062414	-2.657447	2.160736
17	6	3.238563	-1.242841	-1.345571
18	6	3.760909	-1.124809	0.081104
19	6	-3.113240	0.871809	-1.343322
20	6	3.109841	0.885126	1.342484
21	6	2.800354	1.812602	0.187918
22	6	-2.807649	1.801111	-0.189191
23	6	1.372707	2.285547	-1.589548
24	6	2.059770	3.456906	-1.900076
25	6	3.172267	3.792816	-1.129280
26	6	3.558803	2.954624	-0.081871
27	6	-3.570795	2.940132	0.080058
28	6	-3.187636	3.780430	1.127026
29	6	-2.073722	3.449485	1.897932
30	6	-1.381838	2.280829	1.587936
31	58	0.000941	-0.492810	-0.000234
32	1	-4.011045	-2.148926	-0.420518
33	1	-4.694702	-0.569071	-0.066356
34	1	-3.946523	-1.844296	1.937571
35	1	-3.108404	-0.278379	1.826237
36	1	-2.172396	-0.723357	-3.022828
37	1	-3.752058	-1.482667	-2.713925
38	1	-2.063898	-3.162384	-3.139579
39	1	-2.548146	-3.328114	-1.442559
40	1	-0.039821	-3.631652	-3.339198
41	1	0.537788	-4.137392	-1.731252
42	1	1.329431	-1.580987	-3.247441
43	1	2.343798	-3.042014	-3.022771

44	1	0.054772	-3.617627	3.349773
45	1	-0.524483	-4.135970	1.746410
46	1	-2.331064	-3.037044	3.032782
47	1	-1.320363	-1.571879	3.247386
48	1	2.177168	-0.714300	3.022698
49	1	3.759225	-1.467896	2.712333
50	1	2.560010	-3.315904	1.439131
51	1	2.078458	-3.154920	3.137350
52	1	3.106252	-0.269277	-1.827872
53	1	3.952684	-1.830867	-1.937539
54	1	4.022980	-2.130567	0.420936
55	1	4.696274	-0.547133	0.063102
56	1	-4.168762	0.979495	-1.639472
57	1	-2.495263	1.177966	-2.193749
58	1	4.164855	0.997586	1.638678
59	1	2.490433	1.188785	2.192759
60	1	1.717126	4.060710	-2.732509
61	1	3.742961	4.690904	-1.347288
62	1	4.431534	3.183166	0.521968
63	1	-4.444490	3.164752	-0.523855
64	1	-3.762005	4.676272	1.344620
65	1	-1.733553	4.055126	2.730048
66	7	-1.731347	1.493637	0.553327
67	7	1.725389	1.500271	-0.554548
68	6	0.186794	1.798947	-2.413407
69	8	-0.165347	0.572542	-2.147317
70	8	-0.338139	2.552777	-3.222963
71	6	-0.193940	1.799465	2.411988
72	8	0.163207	0.574399	2.146428
73	8	0.327830	2.555765	3.221290

E(RB3LYP) =-1864.331053 Hartree
Corrección de punto cero = 0.603947
Suma de las entalpías electrónicas y térmicas = -1863.690452
Suma de las energías libres y térmicas = -1863.794146

[Ce(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.644370	-0.994842	-0.747565
2	7	2.968322	-0.601036	0.506232
3	8	1.668689	-2.087419	-1.583362
4	6	3.073003	-2.264841	-1.354277
5	6	3.355730	-1.515816	1.605580
6	6	2.284486	-1.677508	2.663201
7	8	1.110362	-2.242407	2.045155
8	6	0.156948	-2.616644	3.040650
9	6	-1.087056	-3.140981	2.368723
10	8	-1.665036	-2.087767	1.585547
11	8	-1.106214	-2.246306	-2.043518
12	6	-0.152137	-2.621446	-3.038038
13	6	1.092321	-3.142919	-2.364688
14	7	-2.967202	-0.606661	-0.506916
15	6	-3.352833	-1.522483	-1.606004
16	6	-2.280712	-1.683512	-2.662837
17	6	-3.068499	-2.269476	1.354507
18	6	-3.642858	-1.001318	0.746829
19	6	3.311905	0.796008	0.869360

20	6	-3.312997	0.789696	-0.870562
21	6	-2.788750	1.795527	0.130921
22	6	2.785561	1.800709	-0.132155
23	6	-1.119356	2.326684	1.661586
24	6	-1.725771	3.537961	1.985871
25	6	-2.917730	3.870949	1.343736
26	6	-3.467090	2.982921	0.417573
27	6	3.461487	2.989421	-0.419044
28	6	2.910168	3.876262	-1.345188
29	6	1.718728	3.540861	-1.987046
30	6	1.114826	2.328383	-1.662563
31	58	0.000642	-0.514970	-0.000084
32	1	4.403277	0.914291	0.970271
33	1	2.858465	1.008175	1.842646
34	1	-4.404528	0.906132	-0.971926
35	1	-2.859550	1.002366	-1.843738
36	1	-1.259150	4.174839	2.728512
37	1	-3.425641	4.803406	1.572224
38	1	-4.407462	3.205550	-0.077045
39	1	4.401516	3.213975	0.075354
40	1	3.416178	4.809703	-1.573872
41	1	1.250697	4.176789	-2.729615
42	7	1.627694	1.494474	-0.739362
43	7	-1.630359	1.491650	0.738351
44	6	0.156937	1.855365	2.342418
45	8	0.496752	0.636184	2.026392
46	8	0.758656	2.606144	3.098328
47	6	-0.160659	1.854306	-2.342995
48	8	-0.497382	0.634188	-2.027247
49	8	-0.764535	2.603926	-3.098335
50	1	4.728380	-1.136665	-0.597206
51	1	3.574266	-2.450505	-2.313517
52	1	3.229510	-3.147470	-0.720539
53	1	-4.726427	-1.145984	0.596030
54	1	-3.519704	-0.192947	1.470783
55	1	-3.570514	-2.456569	2.313074
56	1	-3.221423	-3.152632	0.720621
57	1	-2.007286	-0.732961	-3.129325
58	1	-2.645228	-2.378508	-3.431714
59	1	-3.558917	-2.509611	-1.185729
60	1	-4.283071	-1.183964	-2.089308
61	1	2.650461	-2.371382	3.432405
62	1	2.010068	-0.726973	3.129147
63	1	4.285877	-1.175913	2.088098
64	1	3.562699	-2.502930	1.185733
65	1	0.871108	-4.005945	-1.721310
66	1	1.802550	-3.460573	-3.138639
67	1	0.093844	-1.750558	-3.659633
68	1	-0.572835	-3.408704	-3.679951
69	1	3.518759	-0.187197	-1.471911
70	1	-1.796640	-3.457948	3.143564
71	1	-0.864987	-4.005045	1.727015
72	1	0.578710	-3.402121	3.684047
73	1	-0.089876	-1.744783	3.660533

E(RB3LYP) =-1864.3357459 Hartree
Corrección de punto cero = 0.604817
Suma de las entalpías electrónicas y térmicas = -1863.694666
Suma de las energías libres y térmicas = -1863.795877

[Ce(dpa18c6)]$^{+}$ (agua) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.642951	-0.859400	-0.811607
2	7	2.974013	-0.520421	0.465472
3	8	1.693824	-2.043412	-1.580129
4	6	3.119081	-2.145060	-1.420711
5	6	3.408417	-1.455399	1.532110
6	6	2.357125	-1.665614	2.598686
7	8	1.174103	-2.205363	1.975782
8	6	0.274919	-2.716972	2.965830
9	6	-0.969649	-3.217989	2.284559
10	8	-1.581567	-2.116333	1.591401
11	8	-1.051855	-2.280368	-1.963824
12	6	-0.127084	-2.767399	-2.942686
13	6	1.141324	-3.189160	-2.251466
14	7	-2.942240	-0.681532	-0.472350
15	6	-3.322921	-1.639181	-1.539087
16	6	-2.255414	-1.802127	-2.597860
17	6	-2.996277	-2.306170	1.418797
18	6	-3.594336	-1.056356	0.803564
19	6	3.299743	0.868193	0.861427
20	6	-3.340928	0.687297	-0.870409
21	6	-2.824289	1.737639	0.086254
22	6	2.725782	1.888541	-0.095067
23	6	-1.185580	2.342550	1.618364
24	6	-1.822319	3.547525	1.905239
25	6	-3.010740	3.844310	1.236253
26	6	-3.530947	2.919804	0.331461
27	6	3.365546	3.107955	-0.341460
28	6	2.792369	4.002906	-1.244053
29	6	1.620547	3.641276	-1.910577
30	6	1.053354	2.401899	-1.624456
31	58	0.017114	-0.537431	-0.000100
32	1	4.390532	1.009814	0.934163
33	1	2.874180	1.038966	1.854962
34	1	-4.437579	0.770453	-0.945339
35	1	-2.923032	0.879496	-1.863333
36	1	-1.393547	4.216840	2.645492
37	1	-3.541257	4.774192	1.436976
38	1	-4.478064	3.101349	-0.173995
39	1	4.302072	3.341815	0.162259
40	1	3.269954	4.960987	-1.445085
41	1	1.153561	4.285801	-2.649867
42	7	1.579464	1.563162	-0.713095
43	7	-1.662345	1.476104	0.705696
44	6	0.065587	1.893702	2.355854
45	8	0.469825	0.704139	2.055252
46	8	0.586402	2.654320	3.179162
47	6	-0.170913	1.882109	-2.360338
48	8	-0.505869	0.671700	-2.058107
49	8	-0.736348	2.610808	-3.183221
50	1	4.734285	-0.952064	-0.680448
51	1	3.580429	-2.283391	-2.407629
52	1	3.350493	-3.029546	-0.813513
53	1	-4.677720	-1.214778	0.669041
54	1	-3.469264	-0.232111	1.510099
55	1	-3.457076	-2.472099	2.401704

56	1	-3.166452	-3.204394	0.811494
57	1	-2.028934	-0.865725	-3.116974
58	1	-2.594035	-2.548032	-3.329429
59	1	-3.499382	-2.618767	-1.089707
60	1	-4.266125	-1.334526	-2.019839
61	1	2.736627	-2.390282	3.331600
62	1	2.088320	-0.739019	3.115132
63	1	4.339022	-1.103724	2.005235
64	1	3.628613	-2.426697	1.083751
65	1	0.960964	-3.992638	-1.523671
66	1	1.849271	-3.553215	-3.006780
67	1	0.085965	-1.974871	-3.673334
68	1	-0.563145	-3.628363	-3.468487
69	1	3.465371	-0.046290	-1.519752
70	1	-1.657920	-3.603445	3.047480
71	1	-0.747340	-4.025115	1.572536
72	1	0.753937	-3.543415	3.509322
73	1	0.022176	-1.920638	3.679408

Energia libre total en disolución con todos los términos no electrostáticos = -1636.293401 Hartrees

[Pr(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.627473	-0.979013	-0.793277
2	7	2.970821	-0.590850	0.471938
3	8	1.641199	-2.084838	-1.586587
4	6	3.051778	-2.251581	-1.389621
5	6	3.376333	-1.507857	1.562599
6	6	2.314378	-1.684699	2.626665
7	8	1.137666	-2.247299	2.011708
8	6	0.197561	-2.641456	3.011538
9	6	-1.053757	-3.153367	2.344492
10	8	-1.639751	-2.085724	1.586801
11	8	-1.136018	-2.248184	-2.011576
12	6	-0.195664	-2.641944	-3.011325
13	6	1.055939	-3.152979	-2.344147
14	7	-2.970410	-0.592911	-0.471980
15	6	-3.375203	-1.510197	-1.562668
16	6	-2.313030	-1.686325	-2.626636
17	6	-3.050164	-2.253649	1.389619
18	6	-3.626844	-0.981561	0.793202
19	6	3.315015	0.805583	0.834244
20	6	-3.315591	0.803267	-0.834315
21	6	-2.769156	1.807784	0.156084
22	6	2.767858	1.809709	-0.156162
23	6	-1.078024	2.325934	1.666557
24	6	-1.669958	3.542365	1.997404
25	6	-2.866275	3.885376	1.368541
26	6	-3.433819	3.001294	0.449729
27	6	3.431658	3.003701	-0.449803
28	6	2.863472	3.887372	-1.368615
29	6	1.667403	3.543499	-1.997480
30	6	1.076352	2.326635	-1.666642
31	59	0.000189	-0.509278	-0.000016
32	1	4.407496	0.928369	0.916687
33	1	2.878001	1.013340	1.815924

34	1	-4.408157	0.925287	-0.916780
35	1	-2.878705	1.011319	-1.815990
36	1	-1.189865	4.175377	2.734768
37	1	-3.363604	4.822211	1.602307
38	1	-4.378296	3.231083	-0.033649
39	1	4.375969	3.234173	0.033571
40	1	3.360120	4.824567	-1.602378
41	1	1.186850	4.176171	-2.734837
42	7	1.604914	1.495917	-0.749388
43	7	-1.605980	1.494828	0.749304
44	6	0.200189	1.840929	2.332084
45	8	0.520332	0.617172	2.012653
46	8	0.821907	2.583974	3.079384
47	6	-0.201517	1.840691	-2.332153
48	8	-0.520723	0.616679	-2.012756
49	8	-0.823837	2.583306	-3.079379
50	1	4.714772	-1.115422	-0.662603
51	1	3.532217	-2.431906	-2.360439
52	1	3.228961	-3.134085	-0.761313
53	1	-4.714024	-1.118845	0.662454
54	1	-3.484767	-0.173980	1.514542
55	1	-3.530595	-2.434399	2.360361
56	1	-3.226503	-3.136290	0.761265
57	1	-2.039547	-0.741496	-3.104295
58	1	-2.686854	-2.387120	-3.385775
59	1	-3.587905	-2.493099	-1.136026
60	1	-4.305958	-1.164791	-2.039926
61	1	2.688728	-2.385259	3.385762
62	1	2.040329	-0.740052	3.104361
63	1	4.306906	-1.161837	2.039766
64	1	3.589640	-2.490619	1.135938
65	1	0.842333	-4.005131	-1.684065
66	1	1.757168	-3.483564	-3.120773
67	1	0.044258	-1.782347	-3.650751
68	1	-0.625559	-3.439266	-3.634511
69	1	3.484691	-0.171560	-1.514623
70	1	-1.754739	-3.484275	3.121205
71	1	-0.839648	-4.005490	1.684534
72	1	0.627955	-3.438416	3.634843
73	1	-0.042855	-1.781900	3.650830

E(RB3LYP) =-1864.9691819 Hartree
Corrección de punto cero = 0.605052
Suma de las entalpías electrónicas y térmicas = -1864.327929
Suma de las energías libres y térmicas = -1864.428911

[Pr(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.756373	1.105605	-0.009058
2	7	2.801992	0.531781	-0.992883
3	8	1.944294	1.918855	1.332490
4	6	3.200277	1.223660	1.404910
5	6	2.780899	1.322711	-2.244748
6	6	2.096038	2.673858	-2.089695
7	8	0.727085	2.470400	-1.699956
8	6	-0.265707	3.270831	-2.351187
9	6	-1.490949	2.415437	-2.598476

10	8	-1.944633	1.918644	-1.332383
11	8	-0.727507	2.470214	1.700003
12	6	0.265140	3.270628	2.351478
13	6	1.490488	2.415354	2.598658
14	7	-2.802113	0.531248	0.992864
15	6	-2.781163	1.322185	2.244726
16	6	-2.096521	2.673443	2.089663
17	6	-3.200461	1.223174	-1.404903
18	6	-3.756592	1.104898	0.009033
19	6	3.116654	-0.883361	-1.307760
20	6	-3.116508	-0.883954	1.307727
21	6	-2.776096	-1.819510	0.168738
22	6	2.776422	-1.819002	-0.168788
23	6	-1.320884	-2.283562	-1.588281
24	6	-1.987208	-3.466335	-1.899836
25	6	-3.103419	-3.813774	-1.139233
26	6	-3.514810	-2.974134	-0.102694
27	6	3.515350	-2.973496	0.102621
28	6	3.104113	-3.813230	1.139144
29	6	1.987837	-3.466015	1.899753
30	6	1.321292	-2.283360	1.588219
31	59	-0.000042	0.497287	-0.000007
32	1	4.041501	2.108898	-0.337731
33	1	4.682446	0.514332	0.028326
34	1	3.902648	1.806214	2.015965
35	1	3.049556	0.250060	1.881593
36	1	2.221509	0.745011	-2.983178
37	1	3.799586	1.490068	-2.634375
38	1	2.129248	3.190178	-3.055901
39	1	2.582357	3.316743	-1.346944
40	1	0.111693	3.633421	-3.314393
41	1	-0.513510	4.136528	-1.723562
42	1	-1.246799	1.574520	-3.259228
43	1	-2.277336	3.028416	-3.059572
44	1	-0.112370	3.632947	3.314743
45	1	0.512861	4.136503	1.724065
46	1	2.276768	3.028359	3.059898
47	1	1.246430	1.574278	3.259240
48	1	-2.221686	0.744583	2.983168
49	1	-3.799883	1.489376	2.634341
50	1	-2.582903	3.316205	1.346851
51	1	-2.129874	3.189805	3.055840
52	1	-3.049497	0.249638	-1.881642
53	1	-3.902935	1.805609	-2.015952
54	1	-4.041991	2.108098	0.337757
55	1	-4.682514	0.513395	-0.028431
56	1	4.177136	-1.000244	-1.581951
57	1	2.514692	-1.174002	-2.174842
58	1	-4.176967	-1.001043	1.581913
59	1	-2.514491	-1.174490	2.174806
60	1	-1.627343	-4.069587	-2.725393
61	1	-3.658543	-4.721383	-1.358021
62	1	-4.392154	-3.210598	0.491341
63	1	4.392738	-3.209783	-0.491419
64	1	3.659405	-4.720742	1.357915
65	1	1.628085	-4.069348	2.725299
66	7	1.696038	-1.497518	0.561450
67	7	-1.695773	-1.497809	-0.561497
68	6	-0.135743	-1.779913	-2.401778
69	8	0.190640	-0.545790	-2.137426

70	8	0.412840	-2.526830	-3.202159
71	6	0.136059	-1.779948	2.401726
72	8	-0.190569	-0.545889	2.137382
73	8	-0.412362	-2.526972	3.202120

E(RB3LYP) = -1864.9653679 Hartree
Corrección de punto cero = 0.604221
Suma de las entalpías electrónicas y térmicas = -1864.324626
Suma de las energías libres y térmicas = -1864.427261

$[Pr(dpa18c6)]^{+}$ (agua) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.591326	-0.980869	-0.838541
2	7	2.951052	-0.619662	0.446557
3	8	1.590913	-2.093628	-1.584718
4	6	3.013368	-2.246904	-1.439204
5	6	3.365415	-1.570497	1.507119
6	6	2.310404	-1.759951	2.573816
7	8	1.109667	-2.254195	1.947031
8	6	0.200586	-2.755902	2.932598
9	6	-1.067799	-3.192107	2.251015
10	8	-1.640603	-2.051194	1.588040
11	8	-1.161915	-2.235258	-1.941615
12	6	-0.265937	-2.763333	-2.925306
13	6	0.992990	-3.224524	-2.242970
14	7	-2.965286	-0.551758	-0.446827
15	6	-3.400547	-1.492801	-1.507481
16	6	-2.348459	-1.711549	-2.571232
17	6	-3.065497	-2.175481	1.439769
18	6	-3.615762	-0.898285	0.836982
19	6	3.326798	0.756804	0.840239
20	6	-3.307756	0.832986	-0.841284
21	6	-2.734903	1.857597	0.111085
22	6	2.776894	1.793455	-0.112577
23	6	-1.058543	2.380584	1.632084
24	6	-1.635428	3.612964	1.928047
25	6	-2.814127	3.966942	1.269451
26	6	-3.383960	3.070388	0.366213
27	6	3.453457	2.990676	-0.369755
28	6	2.905190	3.897489	-1.276053
29	6	1.720103	3.568334	-1.936091
30	6	1.114424	2.350697	-1.636758
31	59	-0.006200	-0.530389	0.001107
32	1	4.422360	0.862920	0.900713
33	1	2.918078	0.940609	1.838502
34	1	-4.400405	0.964911	-0.903800
35	1	-2.892946	1.006527	-1.838881
36	1	-1.170337	4.257975	2.668197
37	1	-3.299563	4.919605	1.477392
38	1	-4.326070	3.297045	-0.130393
39	1	4.399919	3.197261	0.127327
40	1	3.412351	4.838377	-1.485793
41	1	1.271432	4.221393	-2.679335
42	7	1.616494	1.501918	-0.721175
43	7	-1.581229	1.540693	0.719775
44	6	0.173626	1.867013	2.357687
45	8	0.516774	0.662025	2.042635

46	8	0.736470	2.591444	3.185928
47	6	-0.127892	1.863171	-2.362985
48	8	-0.502259	0.669017	-2.041677
49	8	-0.673709	2.598726	-3.192577
50	1	4.680387	-1.112971	-0.722301
51	1	3.458814	-2.405098	-2.430392
52	1	3.217638	-3.137816	-0.831863
53	1	-4.707157	-1.007291	0.718807
54	1	-3.443164	-0.082507	1.543234
55	1	-3.516128	-2.323721	2.430173
56	1	-3.286682	-3.062616	0.832792
57	1	-2.085550	-0.790225	-3.099699
58	1	-2.723809	-2.448527	-3.293991
59	1	-3.624005	-2.460727	-1.053552
60	1	-4.329842	-1.142436	-1.984000
61	1	2.667972	-2.504877	3.297441
62	1	2.072204	-0.831082	3.100757
63	1	4.304591	-1.243399	1.980681
64	1	3.562490	-2.544441	1.053994
65	1	0.791885	-4.015913	-1.507436
66	1	1.681266	-3.618144	-3.001569
67	1	-0.031280	-1.984698	-3.664209
68	1	-0.738181	-3.611751	-3.440241
69	1	3.434412	-0.162060	-1.544973
70	1	-1.764985	-3.567597	3.010668
71	1	-0.883572	-3.990822	1.518988
72	1	0.652669	-3.612147	3.452566
73	1	-0.016733	-1.968026	3.667006

Energia libre total en disolución con todos los términos no electrostáticos = -1865.010851 Hartrees

[Nd(dpa18c6)]$^{+}$ (vacío) Δ(λλλ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.766539	1.102095	0.054702
2	7	2.822627	0.542767	-0.946970
3	8	1.894086	1.842802	1.377098
4	6	3.187398	1.216181	1.462281
5	6	2.819875	1.351862	-2.187541
6	6	2.124185	2.695973	-1.996020
7	8	0.720075	2.557600	-1.709024
8	6	-0.118521	2.494934	-2.876580
9	6	-1.544471	2.751812	-2.435478
10	8	-1.893897	1.841793	-1.377968
11	8	-0.720173	2.557786	1.708967
12	6	0.118857	2.495393	2.876228
13	6	1.544511	2.752858	2.434542
14	7	-2.822589	0.543043	0.946918
15	6	-2.819847	1.351953	2.187629
16	6	-2.124187	2.696106	1.996393
17	6	-3.187600	1.215888	-1.462471
18	6	-3.766397	1.102657	-0.054684
19	6	3.128707	-0.872613	-1.260203
20	6	-3.128938	-0.872309	1.260057
21	6	-2.748120	-1.805101	0.131057
22	6	2.747979	-1.805233	-0.131028
23	6	-1.256002	-2.252404	-1.598013

24	6	-1.900081	-3.444638	-1.919821
25	6	-3.023399	-3.807777	-1.177271
26	6	-3.464078	-2.971984	-0.150200
27	6	3.464051	-2.971981	0.150491
28	6	3.023546	-3.807519	1.177846
29	6	1.900284	-3.444248	1.920413
30	6	1.256073	-2.252159	1.598323
31	60	-0.000087	0.538413	-0.000047
32	1	4.068568	2.103142	-0.265144
33	1	4.686335	0.501460	0.103072
34	1	3.858594	1.834028	2.069654
35	1	3.074651	0.242784	1.947675
36	1	-3.075513	0.242257	-1.947543
37	1	-3.858641	1.833867	-2.069877
38	1	-4.067580	2.104038	0.264892
39	1	-4.686657	0.502676	-0.102563
40	1	4.194623	-1.002807	-1.505715
41	1	2.547748	-1.155449	-2.143524
42	1	-4.194927	-1.002316	1.505357
43	1	-2.548216	-1.155218	2.143513
44	1	-1.517882	-4.042950	-2.738889
45	1	-3.561196	-4.723976	-1.403356
46	1	-4.347848	-3.219987	0.429485
47	1	4.347784	-3.220076	-0.429211
48	1	3.561445	-4.723606	1.404143
49	1	1.518228	-4.042345	2.739704
50	7	1.659151	-1.468782	0.580323
51	7	-1.659263	-1.468762	-0.580286
52	6	-0.065154	-1.737039	-2.393478
53	8	0.258389	-0.505685	-2.111485
54	8	0.492114	-2.469799	-3.200877
55	6	0.065272	-1.736684	2.393789
56	8	-0.258451	-0.505440	2.111487
57	8	-0.491856	-2.469284	3.201425
58	1	-0.025114	1.509881	-3.345251
59	1	0.180168	3.276637	-3.587208
60	1	-2.210221	2.613914	-3.294253
61	1	-1.656343	3.775108	-2.058258
62	1	0.025965	1.510288	3.344904
63	1	-0.179865	3.276959	3.586991
64	1	1.655652	3.776101	2.056974
65	1	2.210690	2.615599	3.293081
66	1	-2.538287	3.253577	1.153028
67	1	-2.249994	3.309811	2.896621
68	1	-3.844427	1.534230	2.554206
69	1	-2.289487	0.779029	2.950964
70	1	2.250240	3.310051	-2.895960
71	1	2.538049	3.253046	-1.152283
72	1	3.844446	1.534227	-2.554100
73	1	2.289541	0.779051	-2.950980

E(RB3LYP) =-1865.5833824 Hartree
Corrección de punto cero = 0.604928
Suma de las entalpías electrónicas y térmicas = -1864.978454
Suma de las energías libres y térmicas = -1864.943150

[Nd(dpa18c6)]$^{+}$ (vacío) Δ(δδδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z

1	6	3.680025	0.913941	0.591300
2	7	2.917534	0.591301	-0.634739
3	8	1.713735	1.743984	1.681873
4	6	3.075139	2.071088	1.370326
5	6	3.218721	1.573184	-1.704178
6	6	2.006868	1.944930	-2.539715
7	8	1.012539	2.500249	-1.642955
8	6	0.012897	3.299784	-2.291490
9	6	-1.133257	2.441502	-2.796201
10	8	-1.714090	1.743540	-1.682023
11	8	-1.013050	2.500079	1.643010
12	6	-0.013560	3.299762	2.291597
13	6	1.132796	2.441673	2.796171
14	7	-2.917634	0.590744	0.634715
15	6	-3.219048	1.572585	1.704128
16	6	-2.007304	1.944553	2.539720
17	6	-3.075521	2.070449	-1.370390
18	6	-3.680182	0.913203	-0.591335
19	6	3.209471	-0.792776	-1.085545
20	6	-3.209292	-0.793382	1.085553
21	6	-2.722676	-1.818945	0.081363
22	6	2.723040	-1.818416	-0.081342
23	6	-1.156359	-2.319274	-1.568928
24	6	-1.758774	-3.544683	-1.845642
25	6	-2.888514	-3.903464	-1.110926
26	6	-3.391183	-3.023468	-0.150267
27	6	3.391773	-3.022810	0.150307
28	6	2.889269	-3.902890	1.110977
29	6	1.759457	-3.544313	1.845683
30	6	1.156809	-2.319024	1.568947
31	60	-0.000050	0.493913	-0.000009
32	1	0.463348	3.871299	-3.113016
33	1	-0.348530	4.005300	-1.536400
34	1	-0.782956	1.685444	-3.505434
35	1	-1.884665	3.068040	-3.289566
36	1	-0.464106	3.871092	3.113199
37	1	0.347695	4.005434	1.536572
38	1	1.884086	3.068317	3.289579
39	1	0.782685	1.685451	3.505324
40	1	4.289043	-0.930821	-1.259644
41	1	2.689478	-0.951812	-2.035126
42	1	-4.288834	-0.931635	1.259671
43	1	-2.689255	-0.952299	2.035131
44	1	-1.340087	-4.171500	-2.624562
45	1	-3.389708	-4.848749	-1.297887
46	1	-4.290037	-3.263883	0.408967
47	1	4.290675	-3.263060	-0.408921
48	1	3.390642	-4.848075	1.297951
49	1	1.340884	-4.171200	2.624608
50	7	1.614481	-1.499103	0.606470
51	7	-1.614183	-1.499428	-0.606460
52	6	0.043206	-1.808318	-2.356852
53	8	0.377636	-0.579337	-2.067379
54	8	0.594831	-2.540340	-3.167001
55	6	-0.042863	-1.808285	2.356850
56	8	-0.377475	-0.579347	2.067406
57	8	-0.594323	-2.540381	3.167047
58	1	4.732983	1.149033	0.362897
59	1	3.643655	2.202957	2.298885

60	1	3.108861	3.016002	0.811879
61	1	-4.733184	1.148100	-0.362939
62	1	-3.677070	0.035748	-1.240504
63	1	-3.644109	2.202233	-2.298917
64	1	-3.109357	3.015354	-0.811933
65	1	-1.591109	1.077922	3.059732
66	1	-2.296626	2.713331	3.267201
67	1	-3.599521	2.487223	1.240856
68	1	-4.011949	1.200527	2.370542
69	1	2.296001	2.713773	-3.267200
70	1	1.590823	1.078220	-3.059714
71	1	4.011648	1.201255	-2.370633
72	1	3.599067	2.487893	-1.240940
73	1	3.677080	0.036503	1.240492

E(RB3LYP) = -1865.5849485 Hartree
Corrección de punto cero = 0.604768
Suma de las entalpías electrónicas y térmicas = -1864.943978
Suma de las energías libres y térmicas = -1865.045444

[Nd(dpa18c6)]$^{+}$ (vacío) Δ(δλλ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.710723	0.886228	0.337702
2	7	2.831294	0.472900	-0.779795
3	8	1.836248	1.855878	1.521539
4	6	3.212050	2.053804	1.181499
5	6	2.974835	1.306921	-1.992827
6	6	2.265162	2.655398	-1.914216
7	8	0.852425	2.526498	-1.672298
8	6	0.046662	2.494904	-2.864552
9	6	-1.374399	2.823129	-2.472383
10	8	-1.835835	1.856294	-1.521514
11	8	-0.851860	2.526664	1.672329
12	6	-0.046107	2.494865	2.864581
13	6	1.375016	2.822804	2.472411
14	7	-2.831194	0.473521	0.779813
15	6	-2.974557	1.307570	1.992847
16	6	-2.264562	2.655883	1.914263
17	6	-3.211618	2.054469	-1.181531
18	6	-3.710531	0.887021	-0.337695
19	6	3.136801	-0.942652	-1.124382
20	6	-3.137005	-0.941962	1.124399
21	6	-2.688486	-1.888383	0.032083
22	6	2.688078	-1.888980	-0.032070
23	6	-1.154313	-2.288187	-1.671307
24	6	-1.761292	-3.495508	-2.009359
25	6	-2.881850	-3.895891	-1.282039
26	6	-3.364653	-3.075601	-0.261008
27	6	3.363992	-3.076341	0.261026
28	6	2.880994	-3.896536	1.282040
29	6	1.760507	-3.495922	2.009342
30	6	1.153795	-2.288465	1.671294
31	60	0.000060	0.489978	-0.000014
32	1	4.213076	-1.079880	-1.315275
33	1	2.600864	-1.187565	-2.045458
34	1	-4.213310	-1.078958	1.315289
35	1	-2.601124	-1.186984	2.045479

36	1	-1.353306	-4.076480	-2.828453
37	1	-3.388740	-4.826896	-1.518701
38	1	-4.253001	-3.348543	0.300187
39	1	4.252296	-3.349464	-0.300149
40	1	3.387679	-4.827653	1.518702
41	1	1.352383	-4.076815	2.828424
42	7	1.593916	-1.524044	0.655741
43	7	-1.594254	-1.523675	-0.655742
44	6	0.037038	-1.737453	-2.440806
45	8	0.359367	-0.518417	-2.107473
46	8	0.601123	-2.436660	-3.272784
47	6	-0.037429	-1.737455	2.440791
48	8	-0.359475	-0.518351	2.107438
49	8	-0.601694	-2.436531	3.272756
50	1	4.724160	1.130771	-0.022956
51	1	3.811400	2.088139	2.101931
52	1	3.328248	3.025287	0.686094
53	1	-4.723923	1.131783	0.022950
54	1	-3.808444	0.027626	-1.004070
55	1	-3.810927	2.088868	-2.101987
56	1	-3.327667	3.025996	-0.686181
57	1	1.431348	3.826777	2.029003
58	1	2.012003	2.794787	3.366937
59	1	-0.109556	1.505193	3.328832
60	1	-0.398565	3.259772	3.567911
61	1	3.808456	0.026827	1.004096
62	1	-2.011391	2.795249	-3.366909
63	1	-1.430525	3.827110	-2.028969
64	1	0.399280	3.259755	-3.567861
65	1	0.109906	1.505232	-3.328831
66	1	4.037725	1.487551	-2.230888
67	1	2.540475	0.741896	-2.820162
68	1	2.425172	3.194094	-2.856062
69	1	2.649354	3.287950	-1.114121
70	1	-2.648602	3.288536	1.114182
71	1	-2.424438	3.194610	2.856115
72	1	-2.540340	0.742432	2.820181
73	1	-4.037409	1.488441	2.230901

E(RB3LYP) = -1865.5879886 Hartree
Corrección de punto cero = 0.605651
Suma de las entalpías electrónicas y térmicas = -1864.946397
Suma de las energías libres y térmicas = -1865.046246

$[Nd(dpa18c6)]^+$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.754046	1.080262	-0.048049
2	7	-2.810207	0.524658	0.956030
3	8	-1.920507	1.903586	-1.352543
4	6	-3.170385	1.200727	-1.450763
5	6	-2.808507	1.331678	2.196909
6	6	-2.125598	2.682070	2.028701
7	8	-0.750528	2.477188	1.660271
8	6	0.233333	3.271396	2.332821
9	6	1.446346	2.407797	2.608388
10	8	1.920152	1.903878	1.352594
11	8	0.750076	2.477362	-1.660242

12	6	-0.233940	3.271479	-2.332669
13	6	-1.446809	2.407698	-2.608298
14	7	2.810084	0.525195	-0.956059
15	6	2.808233	1.332215	-2.196939
16	6	2.125093	2.682488	-2.028730
17	6	3.170175	1.201269	1.450756
18	6	3.753827	1.080970	0.048023
19	6	-3.118983	-0.888710	1.281602
20	6	3.119097	-0.888121	-1.281643
21	6	2.752694	-1.829112	-0.155546
22	6	-2.752365	-1.829631	0.155515
23	6	1.276502	-2.281859	1.586441
24	6	1.924322	-3.474389	1.899036
25	6	3.041809	-3.833812	1.145633
26	6	3.473550	-2.994793	0.117057
27	6	-3.472999	-2.995444	-0.117113
28	6	-3.041081	-3.834377	-1.145684
29	6	-1.923651	-3.474738	-1.899067
30	6	-1.276059	-2.282090	-1.586455
31	60	-0.000042	0.499949	0.000000
32	1	-4.061685	2.080043	0.271229
33	1	-4.669767	0.474547	-0.101410
34	1	-3.863251	1.778545	-2.076889
35	1	-3.003193	0.227931	-1.923425
36	1	-2.256909	0.766430	2.950683
37	1	-3.832576	1.501451	2.571163
38	1	-2.173441	3.216055	2.984476
39	1	-2.603194	3.309315	1.267449
40	1	-0.162984	3.638791	3.286453
41	1	0.501169	4.133689	1.708888
42	1	1.182741	1.570705	3.266258
43	1	2.228374	3.016344	3.082530
44	1	0.162285	3.639054	-3.286270
45	1	-0.501907	4.133655	-1.708628
46	1	-2.228950	3.016150	-3.082374
47	1	-1.183068	1.570712	-3.266250
48	1	2.256719	0.766872	-2.950704
49	1	3.832267	1.502165	-2.571207
50	1	2.602609	3.309841	-1.267516
51	1	2.172799	3.216454	-2.984523
52	1	3.003190	0.228423	1.923388
53	1	3.862940	1.779204	2.076886
54	1	4.061238	2.080828	-0.271225
55	1	4.669683	0.475453	0.101341
56	1	-4.183057	-1.012066	1.538575
57	1	-2.530165	-1.166957	2.161568
58	1	4.183181	-1.011286	-1.538661
59	1	2.530290	-1.166476	-2.161585
60	1	1.550676	-4.075461	2.720059
61	1	3.582939	-4.749683	1.365034
62	1	4.353526	-3.239582	-0.469672
63	1	-4.352944	-3.240398	0.469595
64	1	-3.582039	-4.750345	-1.365103
65	1	-1.549882	-4.075734	-2.720091
66	7	-1.669053	-1.497782	-0.565417
67	7	1.669336	-1.497467	0.565405
68	6	0.094586	-1.761400	2.392794
69	8	-0.210939	-0.522123	2.126633
70	8	-0.471139	-2.499277	3.189701
71	6	-0.094235	-1.761400	-2.392794

72	8	0.211040	-0.522060	-2.126635
73	8	0.471642	-2.499165	-3.189697

E(RB3LYP) =-1865.5876879 Hartree
Corrección de punto cero = 0.604447
Suma de las entalpías electrónicas y térmicas = -1864.946823
Suma de las energías libres y térmicas = -1865.048820

$[Nd(dpa18c6)]^+$ (vacío) Δ(λλδ)(λλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.662629	0.891710	0.786479
2	7	2.936172	0.608198	-0.484069
3	8	1.740043	2.229931	1.336629
4	6	2.727606	1.349056	1.908502
5	6	3.256476	1.649713	-1.488751
6	6	2.215484	1.808905	-2.578318
7	8	0.997516	2.286595	-1.977183
8	6	0.027843	2.652051	-2.962473
9	6	-1.175179	3.203016	-2.226301
10	8	-1.740656	2.229508	-1.336537
11	8	-0.998158	2.286209	1.977281
12	6	-0.028582	2.651891	2.962581
13	6	1.174267	3.203244	2.226418
14	7	-2.936359	0.607351	0.484089
15	6	-3.256945	1.648734	1.488813
16	6	-2.215995	1.808144	2.578391
17	6	-2.727943	1.348338	-1.908448
18	6	-3.662871	0.890733	-0.786455
19	6	3.243372	-0.749217	-0.992561
20	6	-3.243203	-0.750168	0.992510
21	6	-2.711798	-1.802842	0.043264
22	6	2.712289	-1.802077	-0.043341
23	6	-1.084197	-2.308442	-1.542988
24	6	-1.637302	-3.561541	-1.793844
25	6	-2.778551	-3.930000	-1.080158
26	6	-3.336126	-3.035445	-0.164394
27	6	3.337025	-3.034467	0.164334
28	6	2.779741	-3.929206	1.080097
29	6	1.638363	-3.561121	1.793767
30	6	1.084840	-2.308210	1.542891
31	60	-0.000093	0.581128	-0.000002
32	1	4.426631	1.657242	0.610598
33	1	4.190489	-0.002823	1.131812
34	1	3.299778	1.886127	2.674647
35	1	2.224097	0.499257	2.381339
36	1	-2.224165	0.498687	-2.381262
37	1	-3.300235	1.885244	-2.674617
38	1	-4.427050	1.656084	-0.610553
39	1	-4.190519	-0.003912	-1.131820
40	1	4.327167	-0.886570	-1.137209
41	1	2.756638	-0.875837	-1.964438
42	1	-4.326964	-0.887825	1.137132
43	1	-2.756453	-0.876706	1.964389
44	1	-1.177006	-4.202473	-2.537119
45	1	-3.244995	-4.896190	-1.249267
46	1	-4.242122	-3.286104	0.378544
47	1	4.243109	-3.284828	-0.378599

48	1	3.246509	-4.895238	1.249218
49	1	1.178278	-4.202192	2.537053
50	7	1.596835	-1.469972	0.624812
51	7	-1.596471	-1.470368	-0.624915
52	6	0.116817	-1.769445	-2.305414
53	8	0.359464	-0.507888	-2.064515
54	8	0.751838	-2.503320	-3.050133
55	6	-0.116341	-1.769601	2.305326
56	8	-0.359380	-0.508121	2.064438
57	8	-0.751094	-2.503667	3.050086
58	1	-2.575899	2.559316	3.294676
59	1	-2.005477	0.875547	3.110160
60	1	-4.235018	1.454298	1.960021
61	1	-3.330208	2.603599	0.962974
62	1	2.575191	2.560224	-3.294549
63	1	2.005227	0.876288	-3.110155
64	1	3.329498	2.604577	-0.962878
65	1	4.234593	1.455549	-1.959980
66	1	-0.231207	1.774494	-3.569595
67	1	0.440747	3.427366	-3.623594
68	1	-1.935365	3.553492	-2.934549
69	1	-0.872759	4.043576	-1.594530
70	1	0.230736	1.774373	3.569648
71	1	-0.441702	3.427045	3.623755
72	1	0.871578	4.043723	1.594666
73	1	1.934347	3.553949	2.934666

E(RB3LYP) =-1865.5772382 Hartree
Corrección de punto cero = 0.604989
Suma de las entalpías electrónicas y térmicas = -1864.936151
Suma de las energías libres y térmicas = -1865.036109

[Nd(dpa18c6)]$^{+}$ (vacío) Δ(δδλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.297174	1.914096	-0.209168
2	7	2.327679	1.616937	0.867702
3	8	2.776857	-0.212858	-1.236471
4	6	3.841581	0.704835	-0.960914
5	6	2.940759	1.083015	2.102400
6	6	3.310928	-0.398701	2.065085
7	8	2.159562	-1.179593	1.711713
8	6	1.930629	-2.387633	2.449288
9	6	0.440744	-2.471857	2.736099
10	8	-0.318637	-2.383991	1.522887
11	8	1.165471	-2.418879	-1.475735
12	6	2.573237	-2.553514	-1.710725
13	6	3.116366	-1.224222	-2.197220
14	7	-1.625190	-2.268318	-1.011572
15	6	-1.078801	-2.764078	-2.291437
16	6	0.323744	-3.342111	-2.188554
17	6	-0.701225	-3.621654	0.914115
18	6	-1.875947	-3.338305	-0.019281
19	6	1.587735	2.868337	1.194744
20	6	-2.879634	-1.523355	-1.298186
21	6	-3.299129	-0.646031	-0.139604
22	6	0.681875	3.295907	0.059656
23	6	-2.602492	0.722213	1.607470

24	6	-3.914916	1.006172	1.979878
25	6	-4.949303	0.420498	1.252019
26	6	-4.639797	-0.431230	0.190046
27	6	0.402550	4.635037	-0.222999
28	6	-0.456443	4.938212	-1.281622
29	6	-0.986203	3.904165	-2.052936
30	6	-0.644410	2.594829	-1.722159
31	60	0.267095	-0.249824	-0.033138
32	1	2.202549	1.207427	2.897209
33	1	3.842627	1.655154	2.382328
34	1	3.650292	-0.677665	3.069802
35	1	4.125462	-0.626387	1.370945
36	1	2.481858	-2.366821	3.397081
37	1	2.285361	-3.247976	1.865698
38	1	0.135922	-1.612542	3.337487
39	1	0.198000	-3.397726	3.271852
40	1	2.765903	-3.331004	-2.458407
41	1	3.058218	-2.847430	-0.772352
42	1	4.205344	-1.295699	-2.306559
43	1	2.678939	-0.951686	-3.164755
44	1	-1.043450	-1.906007	-2.964836
45	1	-1.731327	-3.535378	-2.736798
46	1	0.347581	-4.317778	-1.686291
47	1	0.708492	-3.482083	-3.206033
48	1	2.283039	3.685192	1.445481
49	1	0.970184	2.663552	2.073516
50	1	-3.697880	-2.211269	-1.563174
51	1	-2.689688	-0.884366	-2.165949
52	1	-4.087858	1.659812	2.827064
53	1	-5.985834	0.608192	1.516824
54	1	-5.424107	-0.922024	-0.377897
55	1	0.850394	5.422901	0.374697
56	1	-0.693001	5.973177	-1.511043
57	1	-1.641115	4.077461	-2.899087
58	7	0.148005	2.305996	-0.674146
59	7	-2.308434	-0.061589	0.554212
60	6	-1.413023	1.256990	2.393276
61	8	-0.272951	0.728760	2.043520
62	8	-1.588732	2.099945	3.262998
63	6	-1.128206	1.397602	-2.530153
64	8	-0.576344	0.270283	-2.172606
65	8	-1.965539	1.555059	-3.408225
66	1	2.782069	2.545527	-0.935652
67	1	4.154139	2.494098	0.174532
68	1	4.280102	1.060039	-1.902649
69	1	4.632399	0.184278	-0.406590
70	1	-2.179247	-4.277626	-0.510006
71	1	-2.710773	-3.019858	0.610342
72	1	-1.034676	-4.323460	1.689746
73	1	0.155692	-4.068899	0.399009

E(RB3LYP) = -1865.5803152 Hartree
Corrección de punto cero = 0.604414
Suma de las entalpías electrónicas y térmicas = -1864.939381
Suma de las energías libres y térmicas = -1865.042414

[Nd(dpa18c6)]$^{+}$ (vacío) Δ(λδδ)(λδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z

1	6	-3.787210	0.992987	-0.482225
2	7	-2.942791	0.682244	0.705302
3	8	-1.833187	1.836863	-1.603833
4	6	-3.022160	1.054958	-1.802420
5	6	-3.162106	1.673518	1.788532
6	6	-1.930945	1.945099	2.633048
7	8	-0.913618	2.491625	1.758159
8	6	0.113393	3.236809	2.428684
9	6	1.279780	2.353464	2.821621
10	8	1.833226	1.836817	1.603839
11	8	0.913671	2.491608	-1.758152
12	6	-0.113323	3.236821	-2.428672
13	6	-1.279730	2.353504	-2.821613
14	7	2.942812	0.682190	-0.705300
15	6	3.162140	1.673454	-1.788537
16	6	1.930979	1.945058	-2.633047
17	6	3.022190	1.054896	1.802422
18	6	3.787238	0.992921	0.482227
19	6	-3.179537	-0.695132	1.201527
20	6	3.179524	-0.695196	-1.201525
21	6	2.721989	-1.737574	-0.203867
22	6	-2.722026	-1.737521	0.203867
23	6	1.183283	-2.274927	1.460104
24	6	1.778908	-3.512857	1.688876
25	6	2.895365	-3.856375	0.925901
26	6	3.387221	-2.952186	-0.017341
27	6	-3.387279	-2.952122	0.017344
28	6	-2.895441	-3.856321	-0.925896
29	6	-1.778980	-3.512826	-1.688874
30	6	-1.183334	-2.274904	-1.460107
31	60	0.000005	0.601646	-0.000003
32	1	-4.260917	1.965811	-0.329296
33	1	-4.600754	0.262533	-0.590383
34	1	-3.658289	1.546482	-2.550326
35	1	-2.743512	0.068216	-2.181875
36	1	-0.300643	3.740316	3.310132
37	1	0.451439	3.999365	1.720038
38	1	0.961190	1.525437	3.466864
39	1	2.037446	2.950737	3.347035
40	1	0.300723	3.740321	-3.310119
41	1	-0.451352	3.999381	-1.720023
42	1	-2.037382	2.950795	-3.347025
43	1	-0.961160	1.525473	-3.466858
44	1	2.743532	0.068156	2.181875
45	1	3.658325	1.546411	2.550329
46	1	4.260949	1.965744	0.329303
47	1	4.600780	0.262465	0.590382
48	1	-4.245369	-0.848752	1.435454
49	1	-2.608962	-0.829465	2.125459
50	1	4.245352	-0.848840	-1.435454
51	1	2.608945	-0.829514	-2.125457
52	1	1.368806	-4.160714	2.455142
53	1	3.393368	-4.809686	1.077138
54	1	4.273143	-3.182524	-0.600798
55	1	-4.273226	-3.182426	0.600778
56	1	-3.393461	-4.809624	-1.077128
57	1	-1.368888	-4.160692	-2.455137
58	7	-1.629861	-1.429831	-0.513496
59	7	1.629828	-1.429866	0.513493

60	6	0.014154	-1.764264	2.291456
61	8	-0.267832	-0.506798	2.075472
62	8	-0.558924	-2.516563	3.067285
63	6	-0.014193	-1.764262	-2.291461
64	8	0.267814	-0.506800	-2.075478
65	8	0.558867	-2.516571	-3.067294
66	1	2.186979	2.698738	-3.388143
67	1	1.548002	1.046664	-3.123394
68	1	3.986448	1.367152	-2.452545
69	1	3.449127	2.621873	-1.328873
70	1	-2.186935	2.698789	3.388139
71	1	-1.547992	1.046700	3.123404
72	1	-3.449067	2.621942	1.328863
73	1	-3.986425	1.367239	2.452538

E(RB3LYP) = =-1865.5797237 Hartree
Corrección de punto cero = 0.605391
Suma de las entalpías electrónicas y térmicas = -1864.938381
Suma de las energías libres y térmicas = -1865.038167

[Nd(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.612262	0.964772	-0.831537
2	7	-2.972981	0.580675	0.443149
3	8	-1.616779	2.082084	-1.586680
4	6	-3.032262	2.239691	-1.417839
5	6	-3.394294	1.498831	1.526544
6	6	-2.340285	1.688727	2.595828
7	8	-1.161619	2.249540	1.983445
8	6	-0.232484	2.659541	2.986473
9	6	1.024655	3.161266	2.323539
10	8	1.616701	2.081994	1.586805
11	8	1.161518	2.249713	-1.983328
12	6	0.232374	2.659840	-2.986297
13	6	-1.024765	3.161464	-2.323286
14	7	2.972977	0.580812	-0.443171
15	6	3.394220	1.499006	-1.526557
16	6	2.340156	1.688920	-2.595784
17	6	3.032147	2.239798	1.417818
18	6	3.612269	0.964949	0.831495
19	6	-3.317402	-0.815392	0.804014
20	6	3.317459	-0.815234	-0.804052
21	6	2.752375	-1.817972	0.177168
22	6	-2.752289	-1.818094	-0.177226
23	6	1.043724	-2.323884	1.671230
24	6	1.623582	-3.544127	2.008569
25	6	2.823168	-3.896168	1.390801
26	6	3.405591	-3.016265	0.477432
27	6	-3.405438	-3.016428	-0.477476
28	6	-2.822969	-3.896299	-1.390847
29	6	-1.623405	-3.544194	-2.008622
30	6	-1.043618	-2.323914	-1.671294
31	60	-0.000025	0.502968	-0.000020
32	1	-4.410524	-0.942471	0.870616
33	1	-2.894492	-1.019807	1.792531
34	1	4.410589	-0.942270	-0.870643
35	1	2.894571	-1.019652	-1.792576

36	1	1.132618	-4.173012	2.742320
37	1	3.311639	-4.836363	1.629663
38	1	4.353326	-3.252310	0.003564
39	1	-4.353151	-3.252529	-0.003595
40	1	-3.311386	-4.836527	-1.629700
41	1	-1.132409	-4.173060	-2.742368
42	7	-1.585318	-1.497012	-0.758269
43	7	1.585377	-1.496956	0.758198
44	6	-0.235338	-1.826446	2.323919
45	8	-0.540075	-0.600285	1.998187
46	8	-0.872184	-2.560740	3.067060
47	6	0.235417	-1.826399	-2.323976
48	8	0.540049	-0.600204	-1.998273
49	8	0.872334	-2.560666	-3.067082
50	1	-4.702084	1.096926	-0.718187
51	1	-3.494079	2.416399	-2.398272
52	1	-3.226910	3.121556	-0.793989
53	1	4.702071	1.097222	0.718106
54	1	3.454996	0.158094	1.550479
55	1	3.494034	2.416593	2.398203
56	1	3.226610	3.121674	0.793925
57	1	2.066349	0.749373	-3.083343
58	1	2.721546	2.394975	-3.346284
59	1	3.613558	2.477983	-1.094429
60	1	4.324756	1.147051	-1.999305
61	1	-2.721717	2.394761	3.346327
62	1	-2.066495	0.749171	3.083380
63	1	-4.324848	1.146849	1.999237
64	1	-3.613620	2.477818	1.094438
65	1	-0.817396	4.003520	-1.648547
66	1	-1.718976	3.503629	-3.101063
67	1	-0.002693	1.810378	-3.640911
68	1	0.669423	3.465797	-3.593257
69	1	-3.454872	0.157937	-1.550519
70	1	1.718851	3.503334	3.101374
71	1	0.817287	4.003412	1.648912
72	1	-0.669543	3.465418	3.593532
73	1	0.002580	1.809996	3.640979

E(RB3LYP) = -1865.5905824 Hartree
Corrección de punto cero = 0.605253
Suma de las entalpías electrónicas y térmicas = -1864.949177
Suma de las energías libres y térmicas = -1865.049986

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(λλλ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.764045	1.024831	0.203461
2	7	2.855638	0.512608	-0.852372
3	8	1.823046	1.804481	1.400386
4	6	3.099309	1.159566	1.571411
5	6	2.898393	1.364564	-2.058981
6	6	2.198328	2.699138	-1.826978
7	8	0.785243	2.544054	-1.596298
8	6	-0.004708	2.540072	-2.798212
9	6	-1.445662	2.768733	-2.397487
10	8	-1.823113	1.804463	-1.400336
11	8	-0.785327	2.543981	1.596337

12	6	0.004595	2.539971	2.798271
13	6	1.445558	2.768674	2.397598
14	7	-2.855668	0.512485	0.852366
15	6	-2.898454	1.364431	2.058981
16	6	-2.198421	2.699025	1.826993
17	6	-3.099339	1.159483	-1.571402
18	6	-3.764090	1.024684	-0.203465
19	6	3.142546	-0.897572	-1.190789
20	6	-3.142523	-0.897711	1.190767
21	6	-2.691292	-1.836927	0.093732
22	6	2.691362	-1.836819	-0.093760
23	6	-1.150023	-2.242309	-1.600713
24	6	-1.747450	-3.455443	-1.932457
25	6	-2.870671	-3.855304	-1.208412
26	6	-3.360482	-3.029433	-0.196060
27	6	3.360610	-3.029298	0.196024
28	6	2.870835	-3.855202	1.208370
29	6	1.747594	-3.455400	1.932414
30	6	1.150109	-2.242291	1.600680
31	64	-0.000009	0.525123	0.000000
32	1	4.134846	2.010171	-0.093669
33	1	4.648561	0.380378	0.305607
34	1	3.737942	1.770240	2.219280
35	1	2.938675	0.191475	2.052950
36	1	-2.938641	0.191411	-2.052956
37	1	-3.737990	1.770137	-2.219272
38	1	-4.134949	2.009997	0.093683
39	1	-4.648568	0.380185	-0.305638
40	1	4.214959	-1.051434	-1.391198
41	1	2.596097	-1.148173	-2.105072
42	1	-4.214931	-1.051616	1.391168
43	1	-2.596071	-1.148297	2.105052
44	1	-1.332776	-4.040262	-2.745480
45	1	-3.372649	-4.790034	-1.440859
46	1	-4.249247	-3.302399	0.364484
47	1	4.249390	-3.302217	-0.364523
48	1	3.372859	-4.789911	1.440808
49	1	1.332945	-4.040248	2.745430
50	7	1.596095	-1.469893	0.592198
51	7	-1.596044	-1.469943	-0.592222
52	6	0.029683	-1.680546	-2.377316
53	8	0.315064	-0.445791	-2.068579
54	8	0.615304	-2.379342	-3.194686
55	6	-0.029627	-1.680594	2.377283
56	8	-0.315066	-0.445850	2.068558
57	8	-0.615217	-2.379428	3.194643
58	1	0.111441	1.581317	-3.313140
59	1	0.318093	3.359065	-3.454045
60	1	-2.081333	2.671487	-3.283855
61	1	-1.576216	3.770983	-1.972655
62	1	-0.111549	1.581196	3.313161
63	1	-0.318239	3.358934	3.454125
64	1	1.576122	3.770957	1.972850
65	1	2.081202	2.671362	3.283980
66	1	-2.582478	3.209828	0.941316
67	1	-2.352363	3.359251	2.688916
68	1	-3.934261	1.558940	2.385951
69	1	-2.390749	0.825796	2.861542
70	1	2.352238	3.359370	-2.688902
71	1	2.582386	3.209952	-0.941307

72	1	3.934193	1.559101	-2.385958
73	1	2.390692	0.825923	-2.861540

E(RB3LYP) = -1867.9913174 Hartree
Corrección de punto cero = 0.605537
Suma de las entalpías electrónicas y térmicas = -1867.349762
Suma de las energías libres y térmicas = -1867.449809

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(δδδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	1.383468	3.473380	-0.682877
2	7	0.979195	2.793905	0.566595
3	8	1.997010	1.380985	-1.676682
4	6	2.462064	2.715763	-1.436441
5	6	2.009117	2.977441	1.616110
6	6	2.236741	1.730613	2.450489
7	8	2.616765	0.658679	1.550704
8	6	3.255235	-0.446427	2.206904
9	6	2.227259	-1.409896	2.771687
10	8	1.408524	-1.899037	1.697143
11	8	2.310940	-1.418403	-1.486440
12	6	3.323916	-0.580619	-2.059149
13	6	2.720962	0.661344	-2.688465
14	7	0.100811	-2.964982	-0.600976
15	6	1.027176	-3.432576	-1.659030
16	6	1.656631	-2.293197	-2.440215
17	6	1.539087	-3.297105	1.402603
18	6	0.299567	-3.736954	0.643230
19	6	-0.343331	3.287817	1.022574
20	6	-1.310384	-3.037873	-1.048969
21	6	-2.232711	-2.357806	-0.057847
22	6	-1.432451	2.910428	0.039223
23	6	-2.439828	-0.710438	1.573611
24	6	-3.744530	-1.092571	1.874179
25	6	-4.301367	-2.151069	1.156873
26	6	-3.531071	-2.807372	0.195408
27	6	-2.541678	3.721581	-0.211637
28	6	-3.472919	3.319232	-1.170862
29	6	-3.253225	2.143480	-1.888623
30	6	-2.117252	1.395668	-1.590772
31	64	0.462529	-0.065897	-0.005033
32	1	3.921779	-0.079392	2.997763
33	1	3.863308	-0.943907	1.445302
34	1	1.562220	-0.910750	3.481735
35	1	2.726821	-2.241076	3.281441
36	1	3.907629	-1.147005	-2.796071
37	1	3.985114	-0.298624	-1.234300
38	1	3.517167	1.286449	-3.107207
39	1	2.016504	0.409180	-3.486703
40	1	-0.331238	4.381487	1.156494
41	1	-0.558826	2.829544	1.991608
42	1	-1.628731	-4.083803	-1.187112
43	1	-1.384015	-2.531877	-2.015639
44	1	-4.278031	-0.568230	2.658280
45	1	-5.315413	-2.481678	1.360553
46	1	-3.925629	-3.660567	-0.347065
47	1	-2.666427	4.653853	0.329792

48	1	-4.345388	3.933136	-1.373273
49	1	-3.919295	1.799562	-2.671236
50	7	-1.255409	1.756734	-0.624239
51	7	-1.722399	-1.307732	0.605525
52	6	-1.715175	0.380860	2.345404
53	8	-0.454517	0.498830	2.023841
54	8	-2.317969	1.050446	3.172701
55	6	-1.741677	0.138861	-2.359599
56	8	-0.566816	-0.334919	-2.039753
57	8	-2.515892	-0.332687	-3.180607
58	1	1.736426	4.500523	-0.492120
59	1	2.640366	3.220858	-2.393460
60	1	3.412131	2.678578	-0.887787
61	1	0.363542	-4.819670	0.445359
62	1	-0.562108	-3.573814	1.292733
63	1	1.597294	-3.863979	2.339446
64	1	2.462728	-3.472643	0.836276
65	1	0.907151	-1.729664	-2.999045
66	1	2.411773	-2.698222	-3.125373
67	1	1.829664	-4.011595	-1.193901
68	1	0.518370	-4.106883	-2.362741
69	1	3.061326	1.912908	3.150987
70	1	1.336738	1.445444	2.998673
71	1	1.748938	3.810457	2.285519
72	1	2.955136	3.242534	1.137163
73	1	0.509637	3.544274	-1.332426

E(RB3LYP) = -1867.9922703 Hartree
Corrección de punto cero = 0.604999
Suma de las entalpías electrónicas y térmicas = -1867.351047
Suma de las energías libres y térmicas = -1867.452747

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(δλλ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-0.605720	-3.740108	-0.434917
2	7	-0.293124	-2.863512	0.715220
3	8	-1.715247	-1.903393	-1.547063
4	6	-1.792868	-3.307606	-1.285497
5	6	-1.160014	-3.090960	1.889020
6	6	-2.532843	-2.435211	1.775580
7	8	-2.449219	-1.010748	1.591066
8	6	-2.489591	-0.257217	2.816804
9	6	-2.876958	1.159813	2.472704
10	8	-1.924031	1.692854	1.546833
11	8	-2.549290	0.722051	-1.593543
12	6	-2.500607	-0.031520	-2.818851
13	6	-2.722253	-1.483763	-2.474285
14	7	-0.622505	2.810288	-0.714604
15	6	-1.510050	2.938584	-1.887709
16	6	-2.797514	2.127313	-1.776892
17	6	-2.162294	3.079006	1.286176
18	6	-1.032266	3.644670	0.436182
19	6	1.128725	-3.071952	1.094702
20	6	0.765851	3.181105	-1.094680
21	6	1.752074	2.733826	-0.038012
22	6	2.056783	-2.514248	0.037776
23	6	2.210802	1.196598	1.646024

24	6	3.403665	1.832698	1.980107
25	6	3.769351	2.967066	1.255540
26	6	2.925221	3.437125	0.248265
27	6	3.303503	-3.077295	-0.247768
28	6	4.088545	-2.512161	-1.253999
29	6	3.595211	-1.426759	-1.977988
30	6	2.336547	-0.932807	-1.644739
31	64	-0.480867	-0.028420	-0.000510
32	1	1.346503	-4.140576	1.251598
33	1	1.310391	-2.553716	2.039906
34	1	0.859077	4.267780	-1.251131
35	1	1.005270	2.687648	-2.040237
36	1	3.999855	1.437155	2.794419
37	1	4.689245	3.496212	1.486954
38	1	3.166666	4.339048	-0.305701
39	1	3.646988	-3.945588	0.306062
40	1	5.063514	-2.931500	-1.484984
41	1	4.142844	-0.964499	-2.791281
42	7	1.605777	-1.445546	-0.638778
43	7	1.426687	1.620539	0.638874
44	6	1.687453	-0.006555	2.411685
45	8	0.481004	-0.360796	2.064134
46	8	2.389953	-0.552375	3.253012
47	6	1.678314	0.202233	-2.410419
48	8	0.438446	0.414174	-2.064503
49	8	2.314119	0.826160	-3.250486
50	1	-0.773552	-4.780990	-0.110107
51	1	-1.752172	-3.855863	-2.236939
52	1	-2.759949	-3.540126	-0.822726
53	1	-1.317125	4.660101	0.112335
54	1	-0.160681	3.749800	1.085123
55	1	-2.184756	3.627793	2.237922
56	1	-3.149502	3.199503	0.823121
57	1	-3.714747	-1.628846	-2.024964
58	1	-2.657409	-2.086318	-3.390538
59	1	-1.531202	0.115446	-3.304790
60	1	-3.307874	0.296993	-3.485256
61	1	0.272149	-3.746465	-1.083904
62	1	-2.883096	1.765312	3.389305
63	1	-3.879140	1.189697	2.022451
64	1	-3.254326	-0.677144	3.482003
65	1	-1.510433	-0.291839	3.303937
66	1	-1.301693	-4.168469	2.083797
67	1	-0.649065	-2.663044	2.754047
68	1	-3.106949	-2.650200	2.684875
69	1	-3.112673	-2.811613	0.933576
70	1	-3.418520	2.432617	-0.935265
71	1	-3.391125	2.275376	-2.687017
72	1	-0.952847	2.575376	-2.753690
73	1	-1.776286	3.992762	-2.079656

E(RB3LYP) = -1867.9948632 Hartree
Corrección de punto cero = 0.606119
Suma de las entalpías electrónicas y térmicas = -1867.352946
Suma de las energías libres y térmicas = -1867.452256

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z

1	6	-3.734467	-1.056531	0.178921
2	7	-2.824408	-0.534523	-0.871530
3	8	-1.834315	-1.871654	1.385038
4	6	-3.081379	-1.176855	1.550954
5	6	-2.852885	-1.380166	-2.082628
6	6	-2.153337	-2.716087	-1.878166
7	8	-0.770996	-2.485378	-1.550674
8	6	0.202743	-3.279445	-2.238195
9	6	1.375720	-2.394378	-2.599307
10	8	1.879670	-1.831314	-1.381606
11	8	0.830591	-2.464499	1.551276
12	6	-0.122893	-3.275944	2.246995
13	6	-1.315674	-2.416379	2.604964
14	7	2.837367	-0.464641	0.871232
15	6	2.885920	-1.309688	2.082032
16	6	2.218820	-2.661879	1.875955
17	6	3.108570	-1.105469	-1.550225
18	6	3.759766	-0.964316	-0.179253
19	6	-3.134089	0.870022	-1.221653
20	6	3.111935	0.947042	1.221181
21	6	2.666977	1.889673	0.125832
22	6	-2.712483	1.823691	-0.126625
23	6	1.139700	2.283770	-1.584278
24	6	1.727381	3.504299	-1.905499
25	6	2.839211	3.912916	-1.168436
26	6	3.328089	3.088881	-0.153895
27	6	-3.402371	3.006707	0.152583
28	6	-2.933301	3.842910	1.166536
29	6	-1.811748	3.461740	1.903552
30	6	-1.194827	2.255620	1.582890
31	64	0.005545	-0.494357	-0.000496
32	1	-4.084176	-2.050380	-0.115667
33	1	-4.630169	-0.426508	0.270084
34	1	-3.736551	-1.760541	2.210911
35	1	-2.894461	-0.205116	2.017385
36	1	-2.327053	-0.838559	-2.871127
37	1	-3.884984	-1.572608	-2.422719
38	1	-2.217749	-3.291052	-2.808541
39	1	-2.606143	-3.313555	-1.079297
40	1	-0.225921	-3.696125	-3.156644
41	1	0.523032	-4.107542	-1.593395
42	1	1.061675	-1.590931	-3.276004
43	1	2.157430	-2.997985	-3.080025
44	1	0.317518	-3.675717	3.167392
45	1	-0.425056	-4.116115	1.609067
46	1	-2.082398	-3.035579	3.089960
47	1	-1.019671	-1.602178	3.276890
48	1	2.346724	-0.781407	2.870577
49	1	3.922293	-1.477148	2.422357
50	1	2.684333	-3.245929	1.074523
51	1	2.298945	-3.237577	2.804587
52	1	2.896548	-0.140129	-2.019163
53	1	3.777932	-1.673980	-2.209171
54	1	4.137269	-1.947363	0.117382
55	1	4.637643	-0.310187	-0.273549
56	1	-4.207005	1.000592	-1.435183
57	1	-2.582049	1.124869	-2.131659
58	1	4.181272	1.104304	1.434774
59	1	2.553675	1.188216	2.131125

60	1	1.315878	4.087672	-2.721196
61	1	3.334197	4.853244	-1.393189
62	1	4.209207	3.368525	0.415309
63	1	-4.290052	3.264643	-0.416663
64	1	-3.450766	4.771181	1.390771
65	1	-1.414087	4.055397	2.718693
66	7	-1.618999	1.476065	0.570814
67	7	1.582272	1.515347	-0.571595
68	6	-0.021536	1.702619	-2.374789
69	8	-0.270602	0.455177	-2.086726
70	8	-0.624737	2.399904	-3.180776
71	6	-0.019521	1.703085	2.373158
72	8	0.259387	0.461892	2.085519
73	8	0.567040	2.415079	3.178586

E(RB3LYP) = -1867.9956456 Hartree
Corrección de punto cero = 0.604995
Suma de las entalpías electrónicas y térmicas = -1867.354447
Suma de las energías libres y térmicas = -1867.455290

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(λλδ)(λλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	0.935045	3.604372	-0.911443
2	7	0.666458	2.939006	0.391861
3	8	2.177714	1.588240	-1.345892
4	6	1.385568	2.608733	-1.987396
5	6	1.734151	3.267637	1.361470
6	6	1.907507	2.241402	2.461793
7	8	2.337773	1.000907	1.868418
8	6	2.717622	0.051607	2.868004
9	6	3.138124	-1.210840	2.148391
10	8	2.062277	-1.729898	1.352708
11	8	2.268969	-1.156468	-1.862049
12	6	2.723606	-0.233272	-2.855121
13	6	3.223938	0.996156	-2.129863
14	7	0.468493	-2.981401	-0.398196
15	6	1.507372	-3.377840	-1.373845
16	6	1.751903	-2.357848	-2.465660
17	6	1.195865	-2.695329	1.983823
18	6	0.702528	-3.664628	0.902772
19	6	-0.676615	3.277682	0.910027
20	6	-0.896372	-3.226994	-0.911790
21	6	-1.919006	-2.598423	0.010757
22	6	-1.740305	2.719881	-0.011443
23	6	-2.321061	-0.905625	1.555632
24	6	-3.602764	-1.376517	1.825915
25	6	-4.042964	-2.509691	1.140295
26	6	-3.186290	-3.141960	0.237451
27	6	-2.967381	3.348163	-0.239933
28	6	-3.863708	2.774994	-1.143877
29	6	-3.499800	1.615316	-1.830111
30	6	-2.253619	1.058228	-1.557308
31	64	0.566536	-0.018724	0.001357
32	1	1.698390	4.379644	-0.781843
33	1	0.034908	4.110723	-1.272881
34	1	1.991877	3.119340	-2.744197
35	1	0.531583	2.137354	-2.482545

36	1	0.364705	-2.167031	2.459714
37	1	1.753229	-3.239891	2.754506
38	1	1.432227	-4.471108	0.770103
39	1	-0.218877	-4.134162	1.260590
40	1	-0.807497	4.366933	1.014819
41	1	-0.793877	2.829704	1.900973
42	1	-1.101308	-4.304696	-1.016920
43	1	-0.984636	-2.771475	-1.902462
44	1	-4.209393	-0.863076	2.562970
45	1	-5.034272	-2.913514	1.323623
46	1	-3.490782	-4.046107	-0.280222
47	1	-3.210503	4.271154	0.276947
48	1	-4.824943	3.245295	-1.328871
49	1	-4.137813	1.145685	-2.569898
50	7	-1.416371	1.582354	-0.645415
51	7	-1.519339	-1.485515	0.645267
52	6	-1.701482	0.270133	2.291757
53	8	-0.432246	0.434141	2.024049
54	8	-2.380202	0.958166	3.041445
55	6	-1.710710	-0.154190	-2.294411
56	8	-0.454820	-0.399135	-2.025387
57	8	-2.431727	-0.796994	-3.044719
58	1	2.506001	-2.759822	-3.155773
59	1	0.846635	-2.107724	-3.025953
60	1	1.265632	-4.346547	-1.842672
61	1	2.443975	-3.504065	-0.826256
62	1	2.689000	2.594595	3.148182
63	1	0.987509	2.060249	3.024714
64	1	2.676175	3.321591	0.811164
65	1	1.564076	4.255276	1.822218
66	1	1.872149	-0.132781	3.543372
67	1	3.560129	0.444476	3.454688
68	1	3.481178	-1.969156	2.861265
69	1	3.952273	-0.994054	1.450405
70	1	1.899003	0.011860	-3.536874
71	1	3.541609	-0.682520	-3.436015
72	1	4.013832	0.723700	-1.423472
73	1	3.625984	1.728795	-2.838766

E(RB3LYP) = -1867.9831097 Hartree
Corrección de punto cero = 0.605042
Suma de las entalpías electrónicas y térmicas = -1867.341912
Suma de las energías libres y térmicas = -1867.442108

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(δδλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	1.692895	3.350973	-0.438373
2	7	1.103116	2.629684	0.709679
3	8	2.436717	1.222317	-1.302024
4	6	2.792109	2.603387	-1.183086
5	6	1.975087	2.573321	1.900802
6	6	3.062862	1.501362	1.858027
7	8	2.473694	0.214492	1.614143
8	6	2.892100	-0.874924	2.448741
9	6	1.656664	-1.689349	2.790819
10	8	0.964489	-2.080046	1.596394
11	8	2.264575	-1.505987	-1.324162

12	6	3.531556	-0.879725	-1.567699
13	6	3.294579	0.484074	-2.183361
14	7	-0.195805	-2.797549	-0.895005
15	6	0.552985	-2.998210	-2.150378
16	6	2.046627	-2.744368	-2.024643
17	6	1.266583	-3.380412	1.079184
18	6	0.124270	-3.791066	0.154476
19	6	-0.182780	3.289212	1.068825
20	6	-1.648483	-2.821091	-1.201153
21	6	-2.465789	-2.203678	-0.088405
22	6	-1.224392	3.072068	-0.007318
23	6	-2.554995	-0.598253	1.590905
24	6	-3.842674	-0.977190	1.962118
25	6	-4.448041	-2.023584	1.267558
26	6	-3.745179	-2.658808	0.242659
27	6	-2.225588	4.001127	-0.300687
28	6	-3.133853	3.716280	-1.322518
29	6	-2.996999	2.535864	-2.053860
30	6	-1.959966	1.670861	-1.714118
31	64	0.376013	-0.079484	-0.019295
32	1	1.331607	2.342229	2.752010
33	1	2.457840	3.547101	2.094739
34	1	3.564027	1.497446	2.832812
35	1	3.826945	1.688478	1.098389
36	1	3.345733	-0.495970	3.372069
37	1	3.643318	-1.474524	1.917067
38	1	0.951798	-1.071524	3.350308
39	1	1.924144	-2.573256	3.382189
40	1	4.145021	-1.496234	-2.233691
41	1	4.052709	-0.777784	-0.609503
42	1	4.254900	1.001632	-2.300638
43	1	2.813121	0.400523	-3.164890
44	1	0.145698	-2.285955	-2.869003
45	1	0.414742	-4.019312	-2.547283
46	1	2.573826	-3.550580	-1.498254
47	1	2.466924	-2.675894	-3.035195
48	1	-0.042027	4.368632	1.239076
49	1	-0.540347	2.842130	2.000080
50	1	-1.997588	-3.847552	-1.395558
51	1	-1.808720	-2.241253	-2.115308
52	1	-4.324649	-0.458965	2.783196
53	1	-5.447504	-2.356612	1.532093
54	1	-4.178922	-3.495878	-0.295666
55	1	-2.287871	4.929593	0.258476
56	1	-3.925134	4.421761	-1.559132
57	1	-3.652624	2.275396	-2.876941
58	7	-1.123032	1.923259	-0.692935
59	7	-1.899609	-1.178430	0.568741
60	6	-1.781672	0.473251	2.342492
61	8	-0.521469	0.533621	2.012886
62	8	-2.352179	1.175127	3.167563
63	6	-1.664022	0.391755	-2.481061
64	8	-0.538108	-0.168121	-2.133346
65	8	-2.456926	-0.020026	-3.318140
66	1	0.883257	3.538845	-1.145648
67	1	2.091028	4.333550	-0.131700
68	1	2.898643	3.049444	-2.180711
69	1	3.765850	2.683565	-0.682240
70	1	0.351488	-4.778111	-0.280847
71	1	-0.763770	-3.912815	0.779998

72	1	1.319596	-4.098518	1.907787
73	1	2.239783	-3.369646	0.577269

E(RB3LYP) = -1867.9880608 Hartree
Corrección de punto cero = 0.604691
Suma de las entalpías electrónicas y térmicas = -1867.347004
Suma de las energías libres y térmicas = -1867.448562

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(λδδ)(λδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.770629	0.911110	-0.566322
2	7	-2.953939	0.637722	0.647456
3	8	-1.784496	1.815854	-1.576420
4	6	-2.952432	1.026129	-1.851793
5	6	-3.194076	1.654149	1.698859
6	6	-1.965173	1.972467	2.528845
7	8	-0.947585	2.478794	1.628482
8	6	0.062048	3.273934	2.266953
9	6	1.216598	2.419287	2.745184
10	8	1.784292	1.815805	1.576589
11	8	0.947326	2.479033	-1.628229
12	6	-0.062373	3.274308	-2.266418
13	6	-1.216893	2.419735	-2.744851
14	7	2.953885	0.638148	-0.647575
15	6	3.193853	1.654534	-1.699066
16	6	1.964786	1.972842	-2.528816
17	6	2.952403	1.026248	1.851725
18	6	3.770543	0.911706	0.566184
19	6	-3.178463	-0.731187	1.164014
20	6	3.178543	-0.730756	-1.164085
21	6	2.676856	-1.770297	-0.185198
22	6	-2.676635	-1.770659	0.185123
23	6	1.113074	-2.265477	1.467249
24	6	1.678938	-3.514317	1.709422
25	6	2.791412	-3.888425	0.954602
26	6	3.311217	-2.999846	0.011807
27	6	-3.310810	-3.000301	-0.011900
28	6	-2.790889	-3.888770	-0.954735
29	6	-1.678491	-3.514469	-1.709573
30	6	-1.112812	-2.265548	-1.467374
31	64	-0.000039	0.569594	0.000016
32	1	-4.308562	1.852129	-0.425532
33	1	-4.534153	0.135199	-0.711247
34	1	-3.560831	1.531863	-2.612777
35	1	-2.641968	0.055724	-2.247928
36	1	-0.373219	3.838301	3.099803
37	1	0.416603	3.983610	1.513028
38	1	0.883714	1.641607	3.443540
39	1	1.969012	3.049414	3.238731
40	1	0.372827	3.838948	-3.099119
41	1	-0.416932	3.983741	-1.512266
42	1	-1.969371	3.049956	-3.238178
43	1	-0.883992	1.642290	-3.443462
44	1	2.642162	0.055696	2.247669
45	1	3.560748	1.531941	2.612780
46	1	4.308039	1.852986	0.425488
47	1	4.534424	0.136113	0.710960

48	1	-4.246485	-0.905204	1.373167
49	1	-2.629648	-0.841745	2.103848
50	1	4.246581	-0.904656	-1.373252
51	1	2.629730	-0.841388	-2.103913
52	1	1.251698	-4.146409	2.479522
53	1	3.266495	-4.851975	1.114425
54	1	4.197865	-3.251732	-0.561583
55	1	-4.197406	-3.252343	0.561504
56	1	-3.265825	-4.852390	-1.114575
57	1	-1.251173	-4.146474	-2.479700
58	7	-1.582952	-1.436390	-0.518134
59	7	1.583101	-1.436216	0.518039
60	6	-0.043757	-1.715003	2.286810
61	8	-0.297668	-0.456092	2.041876
62	8	-0.634812	-2.434819	3.079406
63	6	0.043931	-1.714868	-2.286918
64	8	0.297672	-0.455937	-2.041908
65	8	0.635065	-2.434549	-3.079577
66	1	2.221921	2.762266	-3.245791
67	1	1.579303	1.100671	-3.061522
68	1	4.009595	1.352309	-2.375514
69	1	3.501873	2.582560	-1.212382
70	1	-2.222489	2.761823	3.245831
71	1	-1.579723	1.100289	3.061565
72	1	-3.501957	2.582162	1.212061
73	1	-4.009972	1.351984	2.375151

E(RB3LYP) = -1867.9869626 Hartree
Corrección de punto cero = 0.605714
Suma de las entalpías electrónicas y térmicas = -1867.345363
Suma de las energías libres y térmicas = -1867.445059

[Gd(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.601131	-0.697393	-0.973658
2	7	3.008103	-0.364177	0.334881
3	8	1.653407	-1.997774	-1.554945
4	6	3.088052	-2.016858	-1.521631
5	6	3.537402	-1.259201	1.387804
6	6	2.534241	-1.544196	2.483854
7	8	1.373689	-2.162168	1.894099
8	6	0.506495	-2.644956	2.918239
9	6	-0.745628	-3.192773	2.286122
10	8	-1.417095	-2.126497	1.598640
11	8	-1.108084	-2.344698	-1.857536
12	6	-0.188768	-2.799712	-2.848136
13	6	1.109244	-3.170508	-2.180130
14	7	-2.946156	-0.712903	-0.358112
15	6	-3.363144	-1.662122	-1.414627
16	6	-2.311531	-1.857739	-2.484379
17	6	-2.831877	-2.351387	1.506718
18	6	-3.506937	-1.113273	0.945748
19	6	3.270073	1.048084	0.692358
20	6	-3.363460	0.660422	-0.718954
21	6	-2.798108	1.691427	0.230890
22	6	2.582423	2.006384	-0.252990
23	6	-1.067918	2.258853	1.675007

24	6	-1.680383	3.456777	2.031911
25	6	-2.907796	3.767368	1.447083
26	6	-3.483966	2.866418	0.550979
27	6	3.121576	3.254651	-0.576127
28	6	2.437115	4.079455	-1.469544
29	6	1.253142	3.623626	-2.049263
30	6	0.790483	2.361178	-1.689546
31	64	0.031336	-0.478618	-0.001169
32	1	4.352915	1.256374	0.702947
33	1	2.886796	1.217261	1.703390
34	1	-4.462794	0.744816	-0.738396
35	1	-2.994470	0.871294	-1.727547
36	1	-1.192994	4.100390	2.755239
37	1	-3.422533	4.689531	1.700621
38	1	-4.453972	3.066268	0.106467
39	1	4.063111	3.568577	-0.136489
40	1	2.836755	5.056265	-1.725937
41	1	0.690371	4.203588	-2.771740
42	7	1.425565	1.587862	-0.789886
43	7	-1.601938	1.413682	0.773796
44	6	0.239596	1.798401	2.291611
45	8	0.571677	0.585074	1.944614
46	8	0.875094	2.541971	3.026617
47	6	-0.450644	1.740871	-2.303445
48	8	-0.623894	0.493679	-1.959422
49	8	-1.178453	2.400063	-3.033263
50	1	4.702973	-0.745619	-0.927219
51	1	3.469063	-2.146774	-2.543137
52	1	3.421783	-2.878171	-0.929358
53	1	-4.592504	-1.304006	0.886533
54	1	-3.359100	-0.293480	1.651875
55	1	-3.229184	-2.544859	2.511819
56	1	-3.014866	-3.245355	0.897194
57	1	-2.078356	-0.930111	-3.013145
58	1	-2.670085	-2.610299	-3.200126
59	1	-3.565209	-2.633905	-0.958807
60	1	-4.302057	-1.336463	-1.888870
61	1	2.983549	-2.243392	3.202697
62	1	2.218799	-0.636862	3.005580
63	1	4.452020	-0.841598	1.837675
64	1	3.819548	-2.212030	0.934709
65	1	0.968512	-3.958369	-1.427835
66	1	1.804257	-3.540781	-2.943387
67	1	-0.014236	-2.004444	-3.584842
68	1	-0.599321	-3.678692	-3.365988
69	1	3.339652	0.092785	-1.680439
70	1	-1.394376	-3.588079	3.077436
71	1	-0.522177	-4.006158	1.582260
72	1	1.006211	-3.441806	3.488067
73	1	0.251785	-1.825590	3.603037

E(RB3LYP) = -1867.995314 Hartree
Corrección de punto cero = 0.605595
Suma de las entalpías electrónicas y térmicas = -1867.353601
Suma de las energías libres y térmicas = -1867.454428

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(λλλ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z

1	6	3.766915	0.986498	0.269095
2	7	2.878273	0.496496	-0.811179
3	8	1.788997	1.761829	1.409484
4	6	3.062042	1.120452	1.617242
5	6	2.935877	1.370117	-1.998471
6	6	2.226872	2.695291	-1.742339
7	8	0.811498	2.526482	-1.533869
8	6	0.041120	2.562045	-2.747497
9	6	-1.405930	2.768043	-2.360604
10	8	-1.789086	1.761746	-1.409480
11	8	-0.811620	2.526442	1.533872
12	6	-0.041246	2.562041	2.747501
13	6	1.405795	2.768108	2.360610
14	7	-2.878304	0.496361	0.811172
15	6	-2.935959	1.369986	1.998460
16	6	-2.227003	2.695189	1.742335
17	6	-3.062094	1.120300	-1.617248
18	6	-3.766970	0.986308	-0.269106
19	6	3.152166	-0.911208	-1.159785
20	6	-3.152125	-0.911355	1.159781
21	6	-2.662548	-1.850421	0.078615
22	6	2.662638	-1.850295	-0.078614
23	6	-1.097694	-2.231229	-1.598960
24	6	-1.672152	-3.452999	-1.938437
25	6	-2.794520	-3.872737	-1.224355
26	6	-3.308046	-3.054440	-0.217844
27	6	3.308195	-3.054284	0.217841
28	6	2.794710	-3.872607	1.224352
29	6	1.672324	-3.452922	1.938436
30	6	1.097805	-2.231178	1.598962
31	67	-0.000012	0.514322	0.000002
32	1	4.162347	1.967458	-0.011171
33	1	4.637655	0.327051	0.391371
34	1	3.677808	1.731028	2.286599
35	1	2.887922	0.151979	2.092164
36	1	-2.887917	0.151837	-2.092169
37	1	-3.677890	1.730842	-2.286609
38	1	-4.162462	1.967244	0.011154
39	1	-4.637668	0.326808	-0.391387
40	1	4.226550	-1.081774	-1.335840
41	1	2.624496	-1.145906	-2.089144
42	1	-4.226502	-1.081975	1.335832
43	1	-2.624449	-1.146022	2.089144
44	1	-1.242071	-4.028453	-2.750151
45	1	-3.278801	-4.815499	-1.461828
46	1	-4.199198	-3.340514	0.332292
47	1	4.199358	-3.340314	-0.332299
48	1	3.279035	-4.815347	1.461822
49	1	1.242271	-4.028397	2.750151
50	7	1.563948	-1.466970	0.593198
51	7	-1.563875	-1.467044	-0.593195
52	6	0.075055	-1.645578	-2.365958
53	8	0.346568	-0.412826	-2.036098
54	8	0.668265	-2.322370	-3.196045
55	6	-0.074966	-1.645581	2.365966
56	8	-0.346542	-0.412846	2.036101
57	8	-0.668144	-2.322403	3.196052
58	1	0.170690	1.623466	-3.294840
59	1	0.369726	3.406095	-3.367626

60	1	-2.028667	2.702861	-3.258877
61	1	-1.547547	3.752211	-1.898268
62	1	-0.170775	1.623457	3.294846
63	1	-0.369893	3.406077	3.367629
64	1	1.547365	3.752282	1.898275
65	1	2.028534	2.702954	3.258884
66	1	-2.597952	3.183843	0.838826
67	1	-2.386947	3.378953	2.584400
68	1	-3.974858	1.577014	2.308080
69	1	-2.440742	0.847628	2.819307
70	1	2.386780	3.379060	-2.584407
71	1	2.597808	3.183961	-0.838833
72	1	3.974764	1.577192	-2.308100
73	1	2.440676	0.847738	-2.819314

E(RB3LYP) = -1869.75073440 Hartree
Corrección de punto cero = 0.605762
Suma de las entalpías electrónicas y térmicas = -1869.109035
Suma de las energías libres y térmicas = -1869.208792

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(δδδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	1.116528	3.572937	-0.682782
2	7	0.769594	2.865205	0.566210
3	8	1.838898	1.522989	-1.688775
4	6	2.230324	2.880188	-1.446363
5	6	1.792891	3.113954	1.606118
6	6	2.124403	1.874579	2.415407
7	8	2.538543	0.837179	1.488139
8	6	3.284993	-0.219147	2.110113
9	6	2.353697	-1.242108	2.732470
10	8	1.523220	-1.794660	1.699068
11	8	2.368823	-1.233976	-1.457607
12	6	3.319522	-0.327912	-2.035037
13	6	2.617378	0.846713	-2.688435
14	7	0.301756	-2.961331	-0.583912
15	6	1.268811	-3.357146	-1.632047
16	6	1.807348	-2.172601	-2.412495
17	6	1.742228	-3.185414	1.426250
18	6	0.542938	-3.715836	0.661394
19	6	-0.582148	3.253936	1.030264
20	6	-1.096757	-3.123921	-1.040356
21	6	-2.060441	-2.492839	-0.056606
22	6	-1.638833	2.785654	0.051417
23	6	-2.366324	-0.856848	1.570528
24	6	-3.645887	-1.315233	1.873006
25	6	-4.138569	-2.406595	1.157808
26	6	-3.329937	-3.018005	0.198058
27	6	-2.808307	3.506311	-0.203025
28	6	-3.702590	3.032788	-1.164946
29	6	-3.388110	1.879249	-1.883063
30	6	-2.198305	1.222739	-1.579650
31	67	0.451240	-0.035409	-0.001440
32	1	3.972354	0.196897	2.857768
33	1	3.876473	-0.683805	1.315025
34	1	1.691268	-0.781713	3.470952
35	1	2.932496	-2.032354	3.223407

36	1	3.954191	-0.859105	-2.755674
37	1	3.947496	0.021952	-1.209847
38	1	3.355042	1.528022	-3.126831
39	1	1.932496	0.519032	-3.476367
40	1	-0.659594	4.346167	1.158893
41	1	-0.757107	2.786510	2.003527
42	1	-1.352839	-4.188204	-1.172208
43	1	-1.198035	-2.630885	-2.011464
44	1	-4.209613	-0.822464	2.656834
45	1	-5.131153	-2.797138	1.362586
46	1	-3.672100	-3.895641	-0.341500
47	1	-3.007212	4.426472	0.337497
48	1	-4.620216	3.576593	-1.369632
49	1	-4.021014	1.484472	-2.669549
50	7	-1.369932	1.647387	-0.609343
51	7	-1.613981	-1.411125	0.603206
52	6	-1.703852	0.277204	2.334219
53	8	-0.455314	0.468321	1.999408
54	8	-2.336066	0.912974	3.166115
55	6	-1.720174	-0.000331	-2.343091
56	8	-0.517740	-0.383378	-2.004334
57	8	-2.441277	-0.529156	-3.177462
58	1	1.410257	4.618886	-0.492081
59	1	2.375073	3.396645	-2.403357
60	1	3.184638	2.895962	-0.902766
61	1	0.687270	-4.791751	0.466949
62	1	-0.334362	-3.616680	1.303407
63	1	1.829735	-3.733799	2.372190
64	1	2.680648	-3.310254	0.869510
65	1	1.021841	-1.678892	-2.986969
66	1	2.606859	-2.513172	-3.082152
67	1	2.113079	-3.865561	-1.157422
68	1	0.823675	-4.075686	-2.336202
69	1	2.960621	2.096892	3.089924
70	1	1.262731	1.527696	2.988882
71	1	1.478095	3.914523	2.292044
72	1	2.710011	3.459343	1.121205
73	1	0.234125	3.596221	-1.324597

E(RB3LYP) = -1869.7515158 Hartree
Corrección de punto cero = 0.605400
Suma de las entalpías electrónicas y térmicas = -1869.110080
Suma de las energías libres y térmicas = -1869.211113

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(δλλ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	0.770081	-3.701156	0.463158
2	7	0.442180	-2.847268	-0.698165
3	8	1.796303	-1.801698	1.546008
4	6	1.924887	-3.208690	1.324484
5	6	1.350519	-3.033243	-1.845275
6	6	2.670571	-2.281630	-1.700696
7	8	2.480464	-0.864327	-1.544774
8	6	2.501120	-0.132453	-2.783917
9	6	2.796332	1.310431	-2.458811
10	8	1.805980	1.792883	-1.545514
11	8	2.484208	0.852049	1.545274

12	6	2.500857	0.120200	2.784499
13	6	2.788764	-1.324210	2.459665
14	7	0.456065	2.845178	0.698020
15	6	1.365036	3.026541	1.845336
16	6	2.681371	2.268358	1.701092
17	6	1.941324	3.199247	-1.324017
18	6	0.788517	3.697331	-0.463259
19	6	-0.959668	-3.120215	-1.103344
20	6	-0.944483	3.125254	1.102863
21	6	-1.910440	2.601966	0.062177
22	6	-1.923081	-2.592503	-0.062536
23	6	-2.265035	1.041727	-1.625068
24	6	-3.500925	1.591969	-1.953960
25	6	-3.945827	2.692563	-1.221440
26	6	-3.133125	3.218709	-0.216091
27	6	-3.148645	-3.203493	0.215791
28	6	-3.958769	-2.673585	1.221233
29	6	-3.508636	-1.575121	1.953758
30	6	-2.270192	-1.030687	1.624820
31	67	0.469652	-0.001133	-0.000055
32	1	-1.131253	-4.198588	-1.251278
33	1	-1.148006	-2.620866	-2.057163
34	1	-1.110662	4.204546	1.250291
35	1	-1.135468	2.627269	2.056864
36	1	-4.068226	1.160604	-2.770715
37	1	-4.902470	3.154814	-1.446908
38	1	-3.435423	4.100040	0.341113
39	1	-3.455168	-4.083316	-0.341487
40	1	-4.917559	-3.131330	1.446776
41	1	-4.073888	-1.141103	2.770528
42	7	-1.518197	-1.507094	0.616826
43	7	-1.510780	1.514572	-0.617104
44	6	-1.652586	-0.111878	-2.398138
45	8	-0.429300	-0.387042	-2.036210
46	8	-2.302467	-0.693278	-3.257333
47	6	-1.652401	0.120104	2.397809
48	8	-0.427843	0.389564	2.035905
49	8	-2.299581	0.704543	3.256980
50	1	0.986428	-4.736965	0.150893
51	1	1.885736	-3.732488	2.289617
52	1	2.907133	-3.422065	0.884258
53	1	1.009702	4.732139	-0.151051
54	1	-0.097808	3.739054	-1.098972
55	1	1.905153	3.723166	-2.289196
56	1	2.924380	3.407885	-0.883342
57	1	3.783783	-1.429818	2.004880
58	1	2.758873	-1.915586	3.384983
59	1	1.536241	0.226699	3.288857
60	1	3.304412	0.502094	3.426302
61	1	-0.116707	-3.738782	1.098478
62	1	2.769910	1.902091	-3.384053
63	1	3.791713	1.410774	-2.003617
64	1	3.302875	-0.518337	-3.425590
65	1	1.536083	-0.233994	-3.288510
66	1	1.571024	-4.100782	-2.020442
67	1	0.837263	-2.652816	-2.730874
68	1	3.288808	-2.468928	-2.586765
69	1	3.246334	-2.601341	-0.833113
70	1	3.258940	2.585113	0.833622
71	1	3.300315	2.452712	2.587291

72	1	0.849677	2.648564	2.730762
73	1	1.590787	4.092960	2.020700

E(RB3LYP) = -1869.75347234 Hartree
Corrección de punto cero = 0.606395
Suma de las entalpías electrónicas y térmicas = -1869.111324
Suma de las energías libres y térmicas = -1869.210514

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.710960	-1.109945	0.230574
2	7	-2.825989	-0.589751	-0.839917
3	8	-1.762035	-1.872695	1.391168
4	6	-3.024304	-1.213902	1.587853
5	6	-2.844242	-1.457663	-2.032687
6	6	-2.105787	-2.767790	-1.802053
7	8	-0.726393	-2.491520	-1.494352
8	6	0.259491	-3.267804	-2.184765
9	6	1.394625	-2.352102	-2.585435
10	8	1.894642	-1.744785	-1.388070
11	8	0.905803	-2.430342	1.494710
12	6	-0.020291	-3.269851	2.194061
13	6	-1.218021	-2.435809	2.591053
14	7	2.861771	-0.381132	0.839876
15	6	2.943290	-1.245684	2.032364
16	6	2.302247	-2.605777	1.799371
17	6	3.104368	-0.994732	-1.586917
18	6	3.782051	-0.835926	-0.230529
19	6	-3.156754	0.804514	-1.202338
20	6	3.089024	1.033486	1.202176
21	6	2.589494	1.964435	0.120274
22	6	-2.726339	1.769607	-0.120671
23	6	1.037978	2.296786	-1.579987
24	6	1.575668	3.538236	-1.907597
25	6	2.672979	3.992876	-1.175648
26	6	3.199862	3.189377	-0.163873
27	6	-3.423636	2.947412	0.162853
28	6	-2.955840	3.787940	1.173574
29	6	-1.828292	3.414462	1.905363
30	6	-1.202568	2.214838	1.578614
31	67	0.017112	-0.486436	-0.000528
32	1	-4.060573	-2.108164	-0.049672
33	1	-4.608871	-0.485516	0.336472
34	1	-3.646072	-1.817371	2.261975
35	1	-2.854846	-0.238465	2.052493
36	1	-2.340888	-0.919322	-2.837779
37	1	-3.873277	-1.687172	-2.359264
38	1	-2.162340	-3.370202	-2.715240
39	1	-2.533773	-3.354621	-0.982137
40	1	-0.172404	-3.717928	-3.085592
41	1	0.618820	-4.071084	-1.529337
42	1	1.043654	-1.576254	-3.275539
43	1	2.190208	-2.939663	-3.063170
44	1	0.444922	-3.680249	3.097258
45	1	-0.322166	-4.102449	1.546246
46	1	-1.968692	-3.076540	3.073094
47	1	-0.923334	-1.632850	3.276468

48	1	2.401674	-0.746087	2.837675
49	1	3.986395	-1.399430	2.358800
50	1	2.769882	-3.157073	0.976431
51	1	2.404404	-3.205466	2.710265
52	1	2.862865	-0.035943	-2.054193
53	1	3.769180	-1.552162	-2.259554
54	1	4.206345	-1.804147	0.051902
55	1	4.630099	-0.145823	-0.339770
56	1	-4.234692	0.923956	-1.397142
57	1	-2.624441	1.056496	-2.124640
58	1	4.155231	1.231578	1.397510
59	1	2.539234	1.245563	2.124287
60	1	1.139447	4.101610	-2.724529
61	1	3.129123	4.951784	-1.404062
62	1	4.073722	3.502859	0.398869
63	1	-4.317989	3.196467	-0.399881
64	1	-3.479871	4.711710	1.401113
65	1	-1.433085	4.008553	2.721392
66	7	-1.623232	1.432595	0.567078
67	7	1.513735	1.548256	-0.567472
68	6	-0.097718	1.664515	-2.365627
69	8	-0.307072	0.414769	-2.054890
70	8	-0.718352	2.323954	-3.189760
71	6	-0.023442	1.667183	2.363776
72	8	0.275077	0.435534	2.053862
73	8	0.548862	2.370429	3.186709

E(RB3LYP) = -1869.75509670 Hartree
Corrección de punto cero = 0.605220
Suma de las entalpías electrónicas y térmicas = -1869.113749
Suma de las energías libres y térmicas = -1869.214332

[Ho(dpa18c6)]$^+$ (vacío) Δ(λλδ)(λλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	0.899583	3.586863	-0.958416
2	7	0.623522	2.953440	0.357680
3	8	2.167277	1.570465	-1.307568
4	6	1.374946	2.561680	-1.995314
5	6	1.680826	3.309250	1.328199
6	6	1.876785	2.284665	2.425391
7	8	2.315595	1.052933	1.824026
8	6	2.752219	0.117347	2.809748
9	6	3.173353	-1.132825	2.070757
10	8	2.080376	-1.671900	1.314054
11	8	2.262168	-1.163348	-1.820386
12	6	2.748496	-0.249998	-2.803755
13	6	3.232782	0.975182	-2.061556
14	7	0.481872	-2.985134	-0.358950
15	6	1.519963	-3.389289	-1.330769
16	6	1.764900	-2.371557	-2.424851
17	6	1.234760	-2.621746	1.996918
18	6	0.727579	-3.628773	0.958055
19	6	-0.723631	3.291007	0.860386
20	6	-0.880188	-3.255745	-0.860738
21	6	-1.903004	-2.611129	0.049553
22	6	-1.776876	2.697565	-0.050016
23	6	-2.308311	-0.895241	1.566559

24	6	-3.584444	-1.370236	1.854372
25	6	-4.022042	-2.516652	1.189363
26	6	-3.166020	-3.158139	0.292684
27	6	-3.012830	3.303485	-0.292199
28	6	-3.897630	2.704413	-1.190437
29	6	-3.514189	1.540017	-1.857664
30	6	-2.261833	1.005170	-1.570329
31	67	0.535121	-0.010854	-0.000449
32	1	1.652658	4.374611	-0.841354
33	1	-0.000603	4.072916	-1.346847
34	1	1.987060	3.050951	-2.761644
35	1	0.532046	2.065760	-2.485517
36	1	0.409521	-2.084208	2.472795
37	1	1.813162	-3.134548	2.773980
38	1	1.453251	-4.442106	0.844492
39	1	-0.191151	-4.083153	1.341909
40	1	-0.867769	4.381408	0.935314
41	1	-0.841015	2.870090	1.863743
42	1	-1.078282	-4.337717	-0.935392
43	1	-0.977180	-2.830101	-1.864354
44	1	-4.189044	-0.850299	2.588753
45	1	-5.009524	-2.924036	1.385768
46	1	-3.466330	-4.073957	-0.206829
47	1	-3.270493	4.231386	0.208855
48	1	-4.864908	3.157993	-1.386134
49	1	-4.142405	1.050315	-2.593012
50	7	-1.434658	1.553671	-0.663048
51	7	-1.507330	-1.483393	0.660461
52	6	-1.688182	0.294275	2.276315
53	8	-0.424509	0.463097	1.982882
54	8	-2.355742	0.987042	3.031005
55	6	-1.697397	-0.211591	-2.280190
56	8	-0.443287	-0.438876	-1.985233
57	8	-2.395636	-0.872465	-3.035675
58	1	2.530932	-2.768210	-3.105310
59	1	0.862772	-2.134873	-2.996040
60	1	1.275950	-4.359392	-1.795769
61	1	2.457244	-3.516714	-0.784396
62	1	2.661005	2.646473	3.104552
63	1	0.964480	2.093394	2.997527
64	1	2.622611	3.388735	0.780577
65	1	1.484540	4.291822	1.789528
66	1	1.937202	-0.088340	3.516316
67	1	3.606044	0.528652	3.367343
68	1	3.563119	-1.887668	2.763228
69	1	3.952935	-0.892885	1.341307
70	1	1.946476	-0.001349	-3.511393
71	1	3.580794	-0.704130	-3.360619
72	1	3.996174	0.693369	-1.330011
73	1	3.664179	1.709364	-2.751532

E(RB3LYP) = -1869.74134251 Hartree
Corrección de punto cero = 0.605250
Suma de las entalpías electrónicas y térmicas = -1869.100005
Suma de las energías libres y térmicas = -1869.200078

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(δδλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z

1	6	1.569655	3.398757	-0.463270
2	7	1.013367	2.662159	0.691140
3	8	2.325546	1.287900	-1.352886
4	6	2.667377	2.671565	-1.228454
5	6	1.895551	2.634777	1.873831
6	6	3.019259	1.602679	1.812295
7	8	2.478343	0.294673	1.562033
8	6	2.920677	-0.775185	2.410910
9	6	1.699140	-1.591197	2.793050
10	8	0.999126	-2.019066	1.616477
11	8	2.300315	-1.446628	-1.269248
12	6	3.528441	-0.759139	-1.547904
13	6	3.204190	0.557904	-2.221550
14	7	-0.120286	-2.805128	-0.865456
15	6	0.644395	-2.998973	-2.110921
16	6	2.126542	-2.691354	-1.972892
17	6	1.341814	-3.318422	1.121282
18	6	0.217893	-3.776244	0.197977
19	6	-0.291218	3.278023	1.055547
20	6	-1.568959	-2.867297	-1.179598
21	6	-2.400723	-2.244239	-0.081501
22	6	-1.328578	3.003556	-0.010939
23	6	-2.514467	-0.628995	1.585574
24	6	-3.796000	-1.023457	1.960374
25	6	-4.387221	-2.081589	1.271451
26	6	-3.674153	-2.714099	0.252187
27	6	-2.366489	3.888026	-0.314886
28	6	-3.258497	3.559262	-1.337704
29	6	-3.068704	2.381357	-2.061145
30	6	-1.999658	1.562149	-1.708937
31	67	0.371863	-0.070338	-0.014363
32	1	1.268448	2.377620	2.729562
33	1	2.346338	3.624017	2.067080
34	1	3.531374	1.608956	2.781053
35	1	3.767842	1.823484	1.046567
36	1	3.393512	-0.375121	3.315100
37	1	3.663228	-1.379703	1.873338
38	1	0.994431	-0.966683	3.344575
39	1	1.982503	-2.457080	3.403508
40	1	4.176433	-1.370061	-2.185505
41	1	4.040981	-0.582404	-0.596594
42	1	4.128947	1.122954	-2.390347
43	1	2.702501	0.400485	-3.183225
44	1	0.219559	-2.312214	-2.843397
45	1	0.545568	-4.029970	-2.493699
46	1	2.677783	-3.478320	-1.442301
47	1	2.552335	-2.608888	-2.979864
48	1	-0.190480	4.364882	1.205469
49	1	-0.624560	2.836230	1.997968
50	1	-1.895752	-3.905023	-1.351414
51	1	-1.739016	-2.313124	-2.107698
52	1	-4.283844	-0.508532	2.780016
53	1	-5.382011	-2.426972	1.537539
54	1	-4.094660	-3.562222	-0.279214
55	1	-2.467258	4.818093	0.235886
56	1	-4.076584	4.230394	-1.582683
57	1	-3.706799	2.090112	-2.887642
58	7	-1.179633	1.852748	-0.684515
59	7	-1.850689	-1.203943	0.565882

60	6	-1.751091	0.451613	2.330702
61	8	-0.496226	0.531098	1.984670
62	8	-2.319309	1.143831	3.165435
63	6	-1.639552	0.296036	-2.465886
64	8	-0.496598	-0.213381	-2.096663
65	8	-2.398414	-0.154087	-3.314831
66	1	0.745334	3.573135	-1.156823
67	1	1.954512	4.387785	-0.160782
68	1	2.754818	3.125263	-2.224521
69	1	3.647141	2.760544	-0.741248
70	1	0.475232	-4.762503	-0.221929
71	1	-0.670432	-3.913675	0.819801
72	1	1.411357	-4.020588	1.962231
73	1	2.317077	-3.286868	0.624686

E(RB3LYP) = -1869.7476164 Hartree
Corrección de punto cero = 0.604978
Suma de las entalpías electrónicas y térmicas = -1869.106320
Suma de las energías libres y térmicas = -1869.208332

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(λδδ)(λδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.769126	0.878396	0.595169
2	7	2.966314	0.616446	-0.628116
3	8	1.762112	1.790536	1.554212
4	6	2.927760	1.010855	1.864950
5	6	3.206507	1.641642	-1.668072
6	6	1.970413	1.979662	-2.479293
7	8	0.956486	2.458466	-1.558441
8	6	-0.046042	3.284335	-2.167759
9	6	-1.196887	2.451908	-2.690976
10	8	-1.762111	1.790539	-1.554210
11	8	-0.956482	2.458461	1.558442
12	6	0.046045	3.284332	2.167759
13	6	1.196888	2.451906	2.690977
14	7	-2.966315	0.616447	0.628117
15	6	-3.206506	1.641644	1.668072
16	6	-1.970412	1.979661	2.479295
17	6	-2.927761	1.010860	-1.864949
18	6	-3.769126	0.878398	-0.595168
19	6	3.182969	-0.749796	-1.148734
20	6	-3.182971	-0.749795	1.148734
21	6	-2.658655	-1.783668	0.175667
22	6	2.658654	-1.783670	-0.175668
23	6	-1.082091	-2.256186	-1.470236
24	6	-1.634828	-3.508488	-1.723101
25	6	-2.746402	-3.898037	-0.974795
26	6	-3.279098	-3.018915	-0.030594
27	6	3.279095	-3.018918	0.030591
28	6	2.746398	-3.898040	0.974790
29	6	1.634825	-3.508490	1.723098
30	6	1.082090	-2.256187	1.470234
31	67	0.000000	0.547691	0.000000
32	1	4.327203	1.808787	0.461019
33	1	4.515636	0.089052	0.754671
34	1	3.518517	1.531272	2.629644
35	1	2.614182	0.045658	2.270741

36	1	0.396797	3.884903	-2.970683
37	1	-0.405808	3.959505	-1.385213
38	1	-0.860719	1.712055	-3.427811
39	1	-1.951008	3.103147	-3.153626
40	1	-0.396795	3.884901	2.970681
41	1	0.405811	3.959501	1.385212
42	1	1.951012	3.103144	3.153628
43	1	0.860718	1.712054	3.427813
44	1	-2.614183	0.045664	-2.270742
45	1	-3.518517	1.531280	-2.629641
46	1	-4.327205	1.808788	-0.461016
47	1	-4.515634	0.089053	-0.754670
48	1	4.251334	-0.936924	-1.345465
49	1	2.644896	-0.852553	-2.095580
50	1	-4.251337	-0.936923	1.345463
51	1	-2.644899	-0.852552	2.095580
52	1	-1.199210	-4.131085	-2.496246
53	1	-3.211491	-4.865217	-1.141866
54	1	-4.166918	-3.281307	0.536248
55	1	4.166915	-3.281308	-0.536252
56	1	3.211486	-4.865221	1.141859
57	1	1.199208	-4.131086	2.496244
58	7	1.562870	-1.436001	0.518292
59	7	-1.562872	-1.436000	-0.518294
60	6	0.070548	-1.687345	-2.280498
61	8	0.316663	-0.430939	-2.012689
62	8	0.666209	-2.387543	-3.086610
63	6	-0.070541	-1.687343	2.280506
64	8	-0.316666	-0.430941	2.012685
65	8	-0.666208	-2.387542	3.086612
66	1	-2.219167	2.789160	3.176440
67	1	-1.583389	1.121129	3.031678
68	1	-4.011364	1.340886	2.358165
69	1	-3.529476	2.560453	1.173676
70	1	2.219171	2.789158	-3.176440
71	1	1.583388	1.121129	-3.031675
72	1	3.529482	2.560451	-1.173677
73	1	4.011363	1.340881	-2.358165

E(RB3LYP) = -1869.74585589 Hartree
Corrección de punto cero = 0.605834
Suma de las entalpías electrónicas y térmicas = -1869.104163
Suma de las energías libres y térmicas = -1869.203876

[Ho(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.586345	-0.590006	-1.031786
2	7	3.021562	-0.274093	0.291830
3	8	1.651413	-1.934777	-1.562158
4	6	3.087361	-1.921272	-1.561667
5	6	3.597808	-1.156316	1.329402
6	6	2.614300	-1.493513	2.428153
7	8	1.467428	-2.132944	1.835885
8	6	0.631566	-2.668925	2.858022
9	6	-0.621605	-3.217280	2.230176
10	8	-1.325969	-2.140448	1.592448
11	8	-1.100487	-2.365844	-1.811782

12	6	-0.187169	-2.815982	-2.808167
13	6	1.129977	-3.135813	-2.153468
14	7	-2.940549	-0.756263	-0.308653
15	6	-3.361269	-1.716858	-1.351664
16	6	-2.318471	-1.908094	-2.430599
17	6	-2.740733	-2.385547	1.549534
18	6	-3.456842	-1.161885	1.010051
19	6	3.246477	1.143236	0.647010
20	6	-3.385418	0.607423	-0.664954
21	6	-2.809055	1.646743	0.268453
22	6	2.506873	2.077129	-0.282820
23	6	-1.062352	2.225707	1.686025
24	6	-1.679161	3.416476	2.057478
25	6	-2.917182	3.719675	1.491031
26	6	-3.499139	2.815727	0.601957
27	6	2.997347	3.341800	-0.620050
28	6	2.272503	4.138019	-1.507196
29	6	1.097997	3.637259	-2.069088
30	6	0.684402	2.362532	-1.694749
31	67	0.040768	-0.459866	-0.000885
32	1	4.321778	1.388070	0.632404
33	1	2.882966	1.299298	1.667554
34	1	-4.485984	0.679124	-0.656354
35	1	-3.046356	0.819698	-1.683830
36	1	-1.187837	4.060242	2.778047
37	1	-3.435683	4.636795	1.754882
38	1	-4.478172	3.007163	0.173857
39	1	3.934686	3.689195	-0.196916
40	1	2.634595	5.126579	-1.774058
41	1	0.507213	4.191677	-2.789268
42	7	1.355855	1.616875	-0.797605
43	7	-1.600749	1.378685	0.788683
44	6	0.253779	1.768816	2.282573
45	8	0.590084	0.563390	1.910918
46	8	0.892527	2.502468	3.024173
47	6	-0.537288	1.691430	-2.289983
48	8	-0.662997	0.444771	-1.922183
49	8	-1.295903	2.310184	-3.023383
50	1	4.690007	-0.613201	-1.018227
51	1	3.446179	-2.049661	-2.591317
52	1	3.452385	-2.771675	-0.972276
53	1	-4.539688	-1.375234	0.984414
54	1	-3.304810	-0.338213	1.710736
55	1	-3.098681	-2.584795	2.568169
56	1	-2.929564	-3.282899	0.947037
57	1	-2.108227	-0.983128	-2.973499
58	1	-2.671568	-2.675287	-3.133730
59	1	-3.548142	-2.687272	-0.886429
60	1	-4.308958	-1.404994	-1.817606
61	1	3.090646	-2.193101	3.129232
62	1	2.277828	-0.606263	2.970786
63	1	4.497531	-0.706077	1.777537
64	1	3.916975	-2.091316	0.863662
65	1	1.023296	-3.909946	-1.381666
66	1	1.823698	-3.503438	-2.918979
67	1	-0.045430	-2.032321	-3.564142
68	1	-0.581044	-3.716533	-3.301892
69	1	3.286286	0.193126	-1.731087
70	1	-1.247949	-3.651980	3.018602
71	1	-0.397948	-4.000993	1.493637

72	1	1.157468	-3.475160	3.390204
73	1	0.373164	-1.880209	3.576618

E(RB3LYP) = -1869.75258776 Hartree
Corrección de punto cero = 0.605704
Suma de las entalpías electrónicas y térmicas = -1869.110766
Suma de las energías libres y térmicas = -1869.211766

[Yb(dpa18c6)]$^+$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.589777	-0.224481	-1.101571
2	7	3.042055	0.043618	0.237970
3	8	1.771626	-1.755724	-1.555932
4	6	3.199958	-1.600802	-1.605410
5	6	3.728176	-0.772881	1.261792
6	6	2.798944	-1.237855	2.361918
7	8	1.718996	-1.982137	1.766534
8	6	0.961124	-2.631346	2.782172
9	6	-0.246968	-3.270335	2.152985
10	8	-1.065045	-2.240187	1.574374
11	8	-0.923115	-2.473281	-1.749820
12	6	0.018831	-2.869654	-2.740835
13	6	1.366176	-3.027621	-2.089897
14	7	-2.869384	-1.011687	-0.255368
15	6	-3.228767	-2.009020	-1.286259
16	6	-2.179459	-2.136801	-2.368992
17	6	-2.454698	-2.608309	1.588943
18	6	-3.300539	-1.457442	1.079169
19	6	3.127015	1.476459	0.584214
20	6	-3.440538	0.305399	-0.599138
21	6	-2.927849	1.392237	0.316361
22	6	2.265649	2.320496	-0.325823
23	6	-1.208752	2.113679	1.700902
24	6	-1.912243	3.251153	2.084182
25	6	-3.180060	3.453320	1.538935
26	6	-3.702865	2.503255	0.661481
27	6	2.609770	3.628613	-0.678712
28	6	1.786790	4.336955	-1.554345
29	6	0.663550	3.708332	-2.091985
30	6	0.396970	2.399614	-1.702642
31	70	0.080971	-0.434694	0.000353
32	1	4.168961	1.835125	0.535716
33	1	2.780924	1.598639	1.615519
34	1	-4.542591	0.284311	-0.556524
35	1	-3.153407	0.542814	-1.628325
36	1	-1.461879	3.932719	2.796682
37	1	-3.765877	4.326390	1.811189
38	1	-4.701957	2.613472	0.251515
39	1	3.513079	4.076716	-0.276720
40	1	2.035345	5.356911	-1.832692
41	1	0.004080	4.189961	-2.804846
42	7	1.159419	1.736311	-0.813453
43	7	-1.691489	1.224590	0.812625
44	6	0.148369	1.760865	2.272509
45	8	0.574658	0.590416	1.881794
46	8	0.738356	2.534938	3.013482
47	6	-0.751727	1.593373	-2.272120

48	8	-0.736832	0.346083	-1.886130
49	8	-1.581028	2.113774	-3.005497
50	1	4.690703	-0.144180	-1.127889
51	1	3.532355	-1.706272	-2.646329
52	1	3.663651	-2.406112	-1.022412
53	1	-4.359022	-1.771202	1.093402
54	1	-3.200874	-0.621470	1.774863
55	1	-2.749650	-2.836716	2.621490
56	1	-2.586346	-3.519973	0.993120
57	1	-2.053025	-1.209985	-2.934160
58	1	-2.469352	-2.947637	-3.051841
59	1	-3.347825	-2.985696	-0.811766
60	1	-4.197360	-1.767941	-1.750677
61	1	3.355138	-1.898429	3.041744
62	1	2.377110	-0.403534	2.928454
63	1	4.569291	-0.222144	1.710991
64	1	4.156725	-1.656613	0.783887
65	1	1.343700	-3.772182	-1.283000
66	1	2.087660	-3.358236	-2.846072
67	1	0.075312	-2.107096	-3.529116
68	1	-0.287593	-3.823953	-3.194467
69	1	3.193838	0.520755	-1.794264
70	1	-0.813169	-3.796683	2.930439
71	1	0.034396	-3.995987	1.377932
72	1	1.571155	-3.403131	3.274532
73	1	0.643627	-1.898124	3.535069

E(RB3LYP) = -1871.49627901 Hartree
Corrección de punto cero = 0.605765
Suma de las entalpías electrónicas y térmicas = -1870.854399
Suma de las energías libres y térmicas = -1870.955605

[Yb(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	0.392512	-3.844585	0.271964
2	7	0.052998	-2.896214	-0.814345
3	8	1.489278	-2.040267	1.396506
4	6	0.621162	-3.164163	1.617557
5	6	0.918439	-3.077754	-1.992701
6	6	2.335789	-2.587427	-1.737715
7	8	2.312926	-1.179648	-1.431501
8	6	3.250588	-0.352605	-2.130752
9	6	2.543986	0.910107	-2.569802
10	8	2.013222	1.528489	-1.391678
11	8	2.549560	0.468539	1.437147
12	6	3.208317	-0.591065	2.140970
13	6	2.166803	-1.596277	2.577974
14	7	0.878723	2.762039	0.813400
15	6	1.761369	2.690730	1.990959
16	6	2.976999	1.811479	1.738512
17	6	1.502587	2.852920	-1.618094
18	6	1.470922	3.574996	-0.274513
19	6	-1.373907	-2.960068	-1.184299
20	6	-0.472045	3.227431	1.183563
21	6	-1.479130	2.875465	0.111008
22	6	-2.240216	-2.333527	-0.114107
23	6	-2.061675	1.392489	-1.581661

24	6	-3.195991	2.126146	-1.915904
25	6	-3.466083	3.285518	-1.188289
26	6	-2.587281	3.677215	-0.177894
27	6	-3.531217	-2.786178	0.173435
28	6	-4.262680	-2.160213	1.183320
29	6	-3.674372	-1.125398	1.911092
30	6	-2.378044	-0.744411	1.577630
31	70	0.474652	-0.069380	0.000444
32	1	1.306958	-4.382354	0.003655
33	1	-0.390843	-4.605918	0.391172
34	1	1.111132	-3.869299	2.301242
35	1	-0.307438	-2.820669	2.081756
36	1	0.492785	-2.490035	-2.808057
37	1	0.965189	-4.133077	-2.313459
38	1	2.936255	-2.753894	-2.638388
39	1	2.818930	-3.112636	-0.906783
40	1	3.634345	-0.874680	-3.014068
41	1	4.093602	-0.117380	-1.469148
42	1	1.730106	0.680776	-3.266975
43	1	3.263941	1.585890	-3.050655
44	1	3.723219	-0.199271	3.024953
45	1	3.949633	-1.059831	1.481882
46	1	2.659049	-2.448203	3.066003
47	1	1.447994	-1.139492	3.267589
48	1	1.185248	2.253129	2.808126
49	1	2.110470	3.688838	2.308199
50	1	3.590191	2.172769	0.906203
51	1	3.600265	1.801101	2.639079
52	1	0.516488	2.785733	-2.086178
53	1	2.175536	3.387159	-2.301122
54	1	2.498107	3.839154	-0.005106
55	1	0.929937	4.523506	-0.396589
56	1	-1.699749	-3.997830	-1.361523
57	1	-1.514951	-2.406972	-2.117809
58	1	-0.490473	4.314613	1.363238
59	1	-0.765680	2.734450	2.115238
60	1	-3.819977	1.785819	-2.734356
61	1	-4.336687	3.892172	-1.420080
62	1	-2.751792	4.594060	0.379680
63	1	-3.949427	-3.618366	-0.384347
64	1	-5.270079	-2.493929	1.414658
65	1	-4.176726	-0.621900	2.729129
66	7	-1.695194	-1.311208	0.565316
67	7	-1.246434	1.740816	-0.568613
68	6	-1.620509	0.167933	-2.362231
69	8	-0.429648	-0.250899	-2.032116
70	8	-2.360820	-0.330779	-3.200307
71	6	-1.608640	0.305661	2.358336
72	8	-0.347431	0.371079	2.030354
73	8	-2.178076	0.989564	3.199260

E(RB3LYP) = -1871.50054964 Hartree
Corrección de punto cero = 0.605551
Suma de las entalpías electrónicas y térmicas = -1870.859019
Suma de las energías libres y térmicas = -1870.959143

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(λλλ)(λλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.772529	-0.944790	-0.345660
2	7	2.911586	-0.477987	0.763139
3	8	1.751161	-1.712832	-1.417576
4	6	3.019652	-1.076728	-1.668579
5	6	2.982588	-1.374489	1.928524
6	6	2.260527	-2.687480	1.648256
7	8	0.843041	-2.503088	1.462320
8	6	0.092559	-2.582288	2.686060
9	6	-1.360576	-2.764654	2.314514
10	8	-1.750567	-1.713403	1.417596
11	8	-0.842186	-2.503385	-1.462305
12	6	-0.091677	-2.582303	-2.686043
13	6	1.361520	-2.764193	-2.314513
14	7	-2.911374	-0.478966	-0.763219
15	6	-2.982049	-1.375483	-1.928603
16	6	-2.259602	-2.688242	-1.648272
17	6	-3.019304	-1.077765	1.668524
18	6	-3.772167	-0.946096	0.345562
19	6	3.169409	0.926974	1.120785
20	6	-3.169630	0.925916	-1.120869
21	6	-2.633263	1.863066	-0.059408
22	6	2.632642	1.863958	0.059378
23	6	-1.038324	2.217107	1.594407
24	6	-1.585397	3.448639	1.942661
25	6	-2.707769	3.890490	1.241996
26	6	-3.250272	3.080338	0.244425
27	6	3.249225	3.081437	-0.244490
28	6	2.706398	3.891411	-1.242030
29	6	1.584147	3.449181	-1.942650
30	6	1.037502	2.217468	-1.594370
31	71	0.000101	-0.499831	0.000024
32	1	4.193336	-1.921388	-0.086651
33	1	4.628214	-0.270650	-0.492178
34	1	3.606648	-1.687624	-2.362588
35	1	2.830431	-0.107596	-2.135175
36	1	-2.830455	-0.108562	2.135120
37	1	-3.606105	-1.688869	2.362516
38	1	-4.192589	-1.922856	0.086529
39	1	-4.628121	-0.272286	0.492050
40	1	4.244885	1.119635	1.266803
41	1	2.665384	1.143803	2.067425
42	1	-4.245154	1.118232	-1.266975
43	1	-2.665586	1.142928	-2.067460
44	1	-1.135778	4.013924	2.750946
45	1	-3.170904	4.842437	1.484951
46	1	-4.144698	3.381054	-0.292450
47	1	4.143578	3.382453	0.292335
48	1	3.169207	4.843508	-1.485014
49	1	1.134311	4.014307	-2.750926
50	7	1.529309	1.461653	-0.594198
51	7	-1.529835	1.461124	0.594221
52	6	0.128284	1.605789	2.347857
53	8	0.383921	0.375893	1.995055
54	8	0.731400	2.258635	3.189826
55	6	-0.128917	1.605744	-2.347787

56	8	-0.384106	0.375757	-1.994982
57	8	-0.732286	2.258383	-3.189737
58	1	0.236711	-1.666758	3.267447
59	1	0.426224	-3.451987	3.266579
60	1	-1.969123	-2.737528	3.224284
61	1	-1.513885	-3.726690	1.810721
62	1	-0.236141	-1.666808	-3.267407
63	1	-0.425051	-3.452101	-3.266583
64	1	1.515169	-3.726186	-1.810742
65	1	1.970053	-2.736828	-3.224285
66	1	-2.616671	-3.155737	-0.728311
67	1	-2.422979	-3.395242	-2.469979
68	1	-4.023264	-1.599233	-2.219311
69	1	-2.502223	-0.869745	-2.768740
70	1	2.424153	-3.394418	2.469968
71	1	2.617708	-3.154881	0.728295
72	1	4.023885	-1.597898	2.219198
73	1	2.502632	-0.868889	2.768669

E(RB3LYP) = -1872.05055844 Hartree
Corrección de punto cero = 0.605921
Suma de las entalpías electrónicas y térmicas = -1871.408774
Suma de las energías libres y térmicas = -1871.508306

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(δδδ)(δδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	2.295903	2.926191	-0.757471
2	7	1.748461	2.404751	0.509242
3	8	2.310682	0.701966	-1.662490
4	6	3.104836	1.884525	-1.507247
5	6	2.809810	2.277878	1.529563
6	6	2.660345	1.032542	2.382278
7	8	2.637342	-0.117174	1.498474
8	6	2.898310	-1.353061	2.181205
9	6	1.618107	-1.914585	2.769028
10	8	0.687095	-2.160543	1.702789
11	8	1.738866	-2.013120	-1.351564
12	6	3.010714	-1.571740	-1.846112
13	6	2.873012	-0.251320	-2.576729
14	7	-0.819697	-2.876253	-0.594403
15	6	-0.052034	-3.586185	-1.638168
16	6	0.927936	-2.678080	-2.358758
17	6	0.446297	-3.547416	1.422307
18	6	-0.858335	-3.656790	0.654652
19	6	0.633214	3.252723	0.984136
20	6	-2.176352	-2.509417	-1.046449
21	6	-2.823962	-1.555478	-0.063594
22	6	-0.534442	3.171904	0.023409
23	6	-2.490165	0.079942	1.555841
24	6	-3.844239	0.124442	1.875628
25	6	-4.712806	-0.707811	1.170205
26	6	-4.195081	-1.574236	0.206370
27	6	-1.381431	4.252000	-0.237137
28	6	-2.386730	4.111741	-1.195800
29	6	-2.493571	2.915554	-1.905591
30	6	-1.607393	1.888563	-1.593353
31	71	0.391713	-0.184517	-0.006458

32	1	3.656304	-1.198927	2.959578
33	1	3.307994	-2.039422	1.433482
34	1	1.146338	-1.198222	3.446366
35	1	1.821515	-2.839871	3.319218
36	1	3.448427	-2.340488	-2.495310
37	1	3.653608	-1.447283	-0.969788
38	1	3.856690	0.083337	-2.924796
39	1	2.206731	-0.332342	-3.441821
40	1	0.948569	4.303850	1.091548
41	1	0.321507	2.892750	1.968586
42	1	-2.816909	-3.399028	-1.166182
43	1	-2.093435	-2.022892	-2.022477
44	1	-4.176440	0.789156	2.664773
45	1	-5.777138	-0.705583	1.386574
46	1	-4.841036	-2.266300	-0.324848
47	1	-1.244806	5.188713	0.294185
48	1	-3.057907	4.939308	-1.406165
49	1	-3.223388	2.761048	-2.692041
50	7	-0.682195	2.004888	-0.624787
51	7	-2.001770	-0.711658	0.583493
52	6	-1.450525	0.889065	2.308559
53	8	-0.224275	0.616548	1.948180
54	8	-1.790036	1.701724	3.156908
55	6	-1.576542	0.569821	-2.342846
56	8	-0.591231	-0.206070	-1.974623
57	8	-2.420479	0.316039	-3.190552
58	1	2.925957	3.817771	-0.597843
59	1	3.365260	2.285394	-2.494963
60	1	4.038654	1.627882	-0.988965
61	1	-1.081326	-4.721221	0.470532
62	1	-1.655477	-3.264689	1.289429
63	1	0.351893	-4.097037	2.366683
64	1	1.293282	-3.966047	0.863066
65	1	0.412134	-1.927356	-2.958707
66	1	1.585658	-3.282985	-2.994747
67	1	0.511790	-4.398549	-1.170046
68	1	-0.716804	-4.052287	-2.379988
69	1	3.529524	0.946948	3.046486
70	1	1.742139	1.055973	2.972075
71	1	2.841227	3.159231	2.188245
72	1	3.778389	2.229248	1.025009
73	1	1.462874	3.228976	-1.393942

E(RB3LYP) = -1872.05071866 Hartree
Corrección de punto cero = 0.605607
Suma de las entalpías electrónicas y térmicas = -1871.409113
Suma de las energías libres y térmicas = -1871.510745

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(δλλ)(δλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-0.245386	-3.779805	0.453506
2	7	-0.315786	-2.869178	-0.706789
3	8	1.232299	-2.207592	1.538182
4	6	0.979079	-3.600221	1.340177
5	6	0.546683	-3.273109	-1.830179
6	6	2.004194	-2.865663	-1.637504
7	8	2.162943	-1.442886	-1.491945

8	6	2.400891	-0.759478	-2.735679
9	6	3.041220	0.566783	-2.415480
10	8	2.185164	1.292015	-1.529644
11	8	2.580805	0.169862	1.501789
12	6	2.433328	-0.532511	2.749450
13	6	2.324449	-2.003504	2.438142
14	7	1.164388	2.645572	0.702073
15	6	2.118306	2.571192	1.821703
16	6	3.166686	1.476709	1.639402
17	6	2.653420	2.629088	-1.339022
18	6	1.673176	3.395916	-0.462919
19	6	-1.729378	-2.755507	-1.136954
20	6	-0.118384	3.248933	1.134281
21	6	-1.190497	2.979570	0.100106
22	6	-2.524571	-1.986124	-0.104135
23	6	-1.905480	1.571537	-1.605743
24	6	-2.963103	2.413090	-1.938172
25	6	-3.131752	3.580096	-1.193396
26	6	-2.222433	3.879947	-0.177805
27	6	-3.870404	-2.246126	0.167929
28	6	-4.510817	-1.529165	1.179926
29	6	-3.781933	-0.604164	1.927107
30	6	-2.443322	-0.408038	1.600238
31	71	0.431938	-0.116550	0.001731
32	1	-2.186996	-3.746623	-1.288219
33	1	-1.762409	-2.226746	-2.092710
34	1	-0.023144	4.335775	1.290060
35	1	-0.409409	2.801839	2.088009
36	1	-3.608673	2.144853	-2.766579
37	1	-3.942847	4.266262	-1.419182
38	1	-2.300530	4.804450	0.385803
39	1	-4.400296	-3.006022	-0.398013
40	1	-5.558143	-1.713997	1.400396
41	1	-4.208896	-0.046709	2.752899
42	7	-1.844853	-1.053815	0.583565
43	7	-1.068248	1.830802	-0.585578
44	6	-1.583370	0.313521	-2.387836
45	8	-0.477696	-0.263475	-2.002533
46	8	-2.332005	-0.075461	-3.274468
47	6	-1.536674	0.519395	2.384846
48	8	-0.289756	0.466947	2.002001
49	8	-1.992816	1.232328	3.268948
50	1	-0.296028	-4.836172	0.138756
51	1	0.779404	-4.073446	2.311698
52	1	1.875294	-4.082681	0.928589
53	1	2.147499	4.343588	-0.155427
54	1	0.813726	3.655393	-1.083535
55	1	2.719693	3.132377	-2.313689
56	1	3.668305	2.607942	-0.920668
57	1	3.251340	-2.373548	1.977090
58	1	2.149979	-2.557988	3.370521
59	1	1.543250	-0.171421	3.272036
60	1	3.323940	-0.371011	3.369018
61	1	-1.125713	-3.589184	1.070118
62	1	3.183425	1.133146	-3.346151
63	1	4.021031	0.421319	-1.938657
64	1	3.096564	-1.345532	-3.348667
65	1	1.455170	-0.624529	-3.268163
66	1	0.505713	-4.362153	-2.008549
67	1	0.168735	-2.779363	-2.728219

68	1	2.591661	-3.208530	-2.497534
69	1	2.450367	-3.305627	-0.746797
70	1	3.777351	1.622969	0.749621
71	1	3.844422	1.478931	2.501386
72	1	1.547103	2.353407	2.726986
73	1	2.637943	3.532326	1.981400

E(RB3LYP) = -1872.05203669 Hartree
Corrección de punto cero = 0.606356
Suma de las entalpías electrónicas y térmicas = -1871.409923
Suma de las energías libres y térmicas = -1871.509275

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(λδλ)(λδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	0.308923	-3.856166	0.286449
2	7	-0.004281	-2.909013	-0.807913
3	8	1.440712	-2.062146	1.395265
4	6	0.552997	-3.168907	1.626359
5	6	0.868312	-3.108639	-1.976671
6	6	2.288564	-2.633088	-1.709600
7	8	2.277739	-1.220747	-1.423319
8	6	3.236410	-0.416313	-2.119536
9	6	2.556906	0.858029	-2.566611
10	8	2.030143	1.489044	-1.393903
11	8	2.549779	0.422727	1.422982
12	6	3.193787	-0.645948	2.125841
13	6	2.138065	-1.632513	2.570060
14	7	0.931565	2.755377	0.807501
15	6	1.823158	2.664352	1.975695
16	6	3.014536	1.756909	1.707948
17	6	1.542741	2.821197	-1.626757
18	6	1.530708	3.552098	-0.287597
19	6	-1.429746	-2.939396	-1.183721
20	6	-0.408680	3.241119	1.184476
21	6	-1.425872	2.899039	0.117855
22	6	-2.282771	-2.286972	-0.117710
23	6	-2.035046	1.423833	-1.572163
24	6	-3.158162	2.174901	-1.905309
25	6	-3.409645	3.338165	-1.177320
26	6	-2.522810	3.716929	-0.169065
27	6	-3.584660	-2.707983	0.169075
28	6	-4.302664	-2.063387	1.176819
29	6	-3.690265	-1.042578	1.904419
30	6	-2.385059	-0.693230	1.571519
31	71	0.468169	-0.077420	-0.000291
32	1	1.208738	-4.421026	0.023789
33	1	-0.494365	-4.595470	0.411424
34	1	1.031464	-3.876790	2.315137
35	1	-0.368498	-2.804811	2.088906
36	1	0.458565	-2.520398	-2.799794
37	1	0.905568	-4.166235	-2.291495
38	1	2.899014	-2.818415	-2.599800
39	1	2.752877	-3.152874	-0.864932
40	1	3.613148	-0.949162	-2.999553
41	1	4.081014	-0.196746	-1.454548
42	1	1.743641	0.641125	-3.268368
43	1	3.292365	1.518842	-3.044793

44	1	3.717281	-0.260725	3.007797
45	1	3.926260	-1.127603	1.466061
46	1	2.620181	-2.494028	3.051328
47	1	1.434974	-1.164577	3.268258
48	1	1.246640	2.239326	2.799338
49	1	2.198576	3.653945	2.289888
50	1	3.619835	2.099151	0.862096
51	1	3.653905	1.736589	2.596870
52	1	0.553221	2.769837	-2.089319
53	1	2.222202	3.338454	-2.316161
54	1	2.563678	3.800742	-0.025273
55	1	1.005281	4.508952	-0.413307
56	1	-1.782142	-3.969136	-1.357522
57	1	-1.554028	-2.386472	-2.119565
58	1	-0.411999	4.329209	1.360034
59	1	-0.703966	2.755709	2.119474
60	1	-3.788137	1.844725	-2.723319
61	1	-4.271439	3.957761	-1.407836
62	1	-2.671495	4.636676	0.388116
63	1	-4.021228	-3.531292	-0.387774
64	1	-5.318049	-2.372602	1.407244
65	1	-4.180485	-0.526635	2.722059
66	7	-1.714342	-1.276397	0.560403
67	7	-1.212699	1.759705	-0.560652
68	6	-1.613751	0.193600	-2.354154
69	8	-0.433736	-0.251340	-2.018708
70	8	-2.358243	-0.286075	-3.199290
71	6	-1.590345	0.336442	2.353290
72	8	-0.329766	0.377897	2.018330
73	8	-2.141392	1.031151	3.197300

E(RB3LYP) = -1872.05492653 Hartree
Corrección de punto cero = 0.605642
Suma de las entalpías electrónicas y térmicas = -1871.413329
Suma de las energías libres y térmicas = -1871.513360

[Lu(dpa18c6)]$^+$ (vacío) Δ(λλδ)(λλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	1.211885	3.470773	-1.028578
2	7	0.887484	2.913850	0.307776
3	8	2.229644	1.306637	-1.311262
4	6	1.557327	2.362843	-2.032513
5	6	1.974913	3.188693	1.267527
6	6	2.092433	2.156811	2.369552
7	8	2.404719	0.885828	1.773338
8	6	2.772003	-0.075552	2.760626
9	6	3.029302	-1.372170	2.028107
10	8	1.855049	-1.793143	1.318146
11	8	2.134012	-1.425923	-1.768888
12	6	2.724351	-0.577125	-2.751135
13	6	3.276775	0.620047	-2.012817
14	7	0.179515	-3.040758	-0.314326
15	6	1.171527	-3.563304	-1.273862
16	6	1.532050	-2.584685	-2.371709
17	6	0.949806	-2.665482	2.030758
18	6	0.361012	-3.660241	1.021465
19	6	-0.423052	3.370688	0.803237

20	6	-1.201232	-3.170636	-0.812607
21	6	-2.145434	-2.401094	0.085219
22	6	-1.522683	2.839231	-0.090373
23	6	-2.358807	-0.630692	1.576329
24	6	-3.673745	-0.966683	1.882706
25	6	-4.234536	-2.070386	1.238059
26	6	-3.456493	-2.810119	0.346475
27	6	-2.702514	3.542040	-0.351823
28	6	-3.633007	3.001828	-1.240593
29	6	-3.345965	1.796493	-1.883211
30	6	-2.145548	1.163443	-1.576519
31	71	0.511911	-0.059210	0.000711
32	1	2.050341	4.171699	-0.947171
33	1	0.367140	4.042946	-1.425294
34	1	2.220750	2.748132	-2.814623
35	1	0.662184	1.950549	-2.505077
36	1	0.172789	-2.056926	2.500171
37	1	1.499815	-3.196874	2.815272
38	1	1.014801	-4.535986	0.940790
39	1	-0.594878	-4.022477	1.413332
40	1	-0.483082	4.470889	0.849835
41	1	-0.569311	2.987191	1.817728
42	1	-1.520127	-4.224876	-0.868700
43	1	-1.251108	-2.754835	-1.823739
44	1	-4.212821	-0.377927	2.616183
45	1	-5.257190	-2.370161	1.447696
46	1	-3.852636	-3.698803	-0.134904
47	1	-2.879865	4.499918	0.127172
48	1	-4.557594	3.531662	-1.450466
49	1	-4.008073	1.348521	-2.615435
50	7	-1.277830	1.655283	-0.673868
51	7	-1.629946	-1.309450	0.672059
52	6	-1.609890	0.493244	2.265042
53	8	-0.343020	0.534826	1.939860
54	8	-2.184800	1.251181	3.032622
55	6	-1.678887	-0.104872	-2.263937
56	8	-0.456362	-0.439768	-1.938577
57	8	-2.414342	-0.708777	-3.031097
58	1	2.266347	-3.060938	-3.036088
59	1	0.666479	-2.267790	-2.960892
60	1	0.828328	-4.504785	-1.735470
61	1	2.086720	-3.787320	-0.721037
62	1	2.917194	2.449060	3.034258
63	1	1.175542	2.056088	2.957653
64	1	2.917511	3.187567	0.715388
65	1	1.864307	4.186420	1.725259
66	1	1.963863	-0.185464	3.496191
67	1	3.682845	0.248895	3.284625
68	1	3.356191	-2.159046	2.716799
69	1	3.804312	-1.228997	1.268893
70	1	1.969309	-0.277246	-3.490147
71	1	3.535353	-1.106880	-3.271804
72	1	3.988809	0.296078	-1.247621
73	1	3.786777	1.307708	-2.696434

E(RB3LYP) = -1872.04012810 Hartree
Corrección de punto cero = 0.605342
Suma de las entalpías electrónicas y térmicas = -1871.398715
Suma de las energías libres y térmicas = -1871.499114

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(δδλ)(δδλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	1.606534	3.371388	-0.519817
2	7	1.065090	2.656655	0.653642
3	8	2.323508	1.231272	-1.365662
4	6	2.677232	2.614569	-1.294880
5	6	1.974966	2.621521	1.812160
6	6	3.058790	1.549083	1.730866
7	8	2.465426	0.256356	1.518501
8	6	2.870434	-0.801222	2.401781
9	6	1.624372	-1.569611	2.799159
10	8	0.917072	-2.004750	1.628815
11	8	2.252861	-1.500817	-1.201768
12	6	3.494221	-0.835435	-1.478465
13	6	3.198971	0.461855	-2.200959
14	7	-0.189510	-2.813047	-0.839075
15	6	0.587150	-3.033831	-2.069926
16	6	2.070204	-2.740985	-1.912361
17	6	1.233330	-3.324579	1.170287
18	6	0.112704	-3.775785	0.240201
19	6	-0.225350	3.286364	1.033979
20	6	-1.633759	-2.834183	-1.165575
21	6	-2.449282	-2.160415	-0.085554
22	6	-1.277299	2.997279	-0.014631
23	6	-2.510416	-0.528773	1.566293
24	6	-3.807824	-0.869382	1.937462
25	6	-4.437749	-1.907278	1.251726
26	6	-3.743192	-2.575340	0.243027
27	6	-2.310938	3.883255	-0.329044
28	6	-3.202221	3.550323	-1.350969
29	6	-3.013268	2.367411	-2.066725
30	6	-1.950830	1.545767	-1.701724
31	71	0.357400	-0.083298	-0.003304
32	1	1.365412	2.401013	2.690574
33	1	2.465607	3.597116	1.976746
34	1	3.606109	1.549440	2.679887
35	1	3.786001	1.731546	0.935660
36	1	3.347619	-0.388391	3.297806
37	1	3.599465	-1.441750	1.887838
38	1	0.937000	-0.911157	3.331691
39	1	1.879624	-2.428918	3.430745
40	1	4.148258	-1.475298	-2.080326
41	1	3.987404	-0.632694	-0.522882
42	1	4.134820	1.006520	-2.377055
43	1	2.706557	0.280163	-3.163233
44	1	0.182105	-2.352400	-2.817936
45	1	0.482892	-4.068761	-2.441040
46	1	2.606229	-3.535231	-1.377052
47	1	2.509189	-2.660684	-2.913706
48	1	-0.118904	4.375796	1.161095
49	1	-0.545047	2.864996	1.990105
50	1	-1.997023	-3.863077	-1.317211
51	1	-1.779958	-2.296182	-2.107189
52	1	-4.277858	-0.330962	2.752396
53	1	-5.447328	-2.210326	1.513555
54	1	-4.192495	-3.411155	-0.284305
55	1	-2.406326	4.819879	0.211483

56	1	-4.016266	4.223354	-1.604014
57	1	-3.645858	2.075660	-2.897290
58	7	-1.135423	1.837146	-0.673862
59	7	-1.862442	-1.135613	0.554266
60	6	-1.706867	0.521817	2.308364
61	8	-0.451883	0.556247	1.953796
62	8	-2.242559	1.233680	3.147680
63	6	-1.581935	0.279308	-2.450728
64	8	-0.448917	-0.234005	-2.055172
65	8	-2.320344	-0.167969	-3.318660
66	1	0.771409	3.550063	-1.198949
67	1	2.012447	4.358333	-0.238407
68	1	2.741776	3.036833	-2.306441
69	1	3.670293	2.712176	-0.836129
70	1	0.356003	-4.773420	-0.161177
71	1	-0.786423	-3.886847	0.851889
72	1	1.271989	-4.006301	2.029640
73	1	2.216694	-3.329977	0.689114

E(RB3LYP) = -1872.04711121 Hartree
Corrección de punto cero = 0.605313
Suma de las entalpías electrónicas y térmicas = -1871.405599
Suma de las energías libres y térmicas = -1871.506815

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(λδδ)(λδδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	-3.771800	0.843984	-0.625892
2	7	-2.985691	0.596811	0.608072
3	8	-1.741494	1.753967	-1.534502
4	6	-2.905233	0.986016	-1.878898
5	6	-3.221375	1.634131	1.632867
6	6	-1.977295	1.988020	2.425121
7	8	-0.963268	2.434784	1.486646
8	6	0.035766	3.282514	2.071416
9	6	1.176062	2.465752	2.639234
10	8	1.741452	1.753992	1.534507
11	8	0.963208	2.434817	-1.486633
12	6	-0.035844	3.282540	-2.071377
13	6	-1.176122	2.465765	-2.639213
14	7	2.985675	0.596896	-0.608101
15	6	3.221327	1.634217	-1.632904
16	6	1.977226	1.988084	-2.425132
17	6	2.905216	0.986068	1.878880
18	6	3.771778	0.844082	0.625864
19	6	-3.190429	-0.765334	1.135685
20	6	3.190416	-0.765248	-1.135714
21	6	2.639865	-1.793746	-0.171102
22	6	-2.639827	-1.793824	0.171091
23	6	1.050434	-2.243019	1.467701
24	6	1.588236	-3.499478	1.730411
25	6	2.697680	-3.905585	0.987706
26	6	3.244277	-3.035743	0.043136
27	6	-3.244208	-3.035833	-0.043162
28	6	-2.697574	-3.905663	-0.987723
29	6	-1.588124	-3.499533	-1.730406
30	6	-1.050352	-2.243064	-1.467682
31	71	-0.000010	0.522850	0.000006

32	1	-4.346918	1.765921	-0.503931
33	1	-4.503264	0.043071	-0.796939
34	1	-3.475788	1.518934	-2.649922
35	1	-2.589208	0.023866	-2.289529
36	1	-0.413415	3.917933	2.843278
37	1	0.407561	3.922206	1.265253
38	1	0.829364	1.761137	3.405224
39	1	1.932183	3.130376	3.078881
40	1	0.413324	3.917983	-2.843224
41	1	-0.407648	3.922206	-1.265196
42	1	-1.932260	3.130384	-3.078842
43	1	-0.829409	1.761177	-3.405220
44	1	2.589217	0.023901	2.289492
45	1	3.475763	1.518982	2.649911
46	1	4.346859	1.766044	0.503915
47	1	4.503276	0.043197	0.796895
48	1	-4.258154	-0.969596	1.320157
49	1	-2.663359	-0.856174	2.089822
50	1	4.258139	-0.969494	-1.320217
51	1	2.663318	-0.856102	-2.089835
52	1	1.144077	-4.112051	2.506713
53	1	3.151281	-4.877121	1.160930
54	1	4.132884	-3.309144	-0.517247
55	1	-4.132821	-3.309254	0.517203
56	1	-3.151151	-4.877209	-1.160956
57	1	-1.143935	-4.112099	-2.506696
58	7	-1.542450	-1.431791	-0.513607
59	7	1.542495	-1.431737	0.513616
60	6	-0.095104	-1.653536	2.270437
61	8	-0.334427	-0.401248	1.976515
62	8	-0.691998	-2.330870	3.094552
63	6	0.095209	-1.653565	-2.270373
64	8	0.334446	-0.401253	-1.976489
65	8	0.692034	-2.330838	-3.094588
66	1	2.215745	2.818374	-3.100868
67	1	1.591850	1.143013	-2.998199
68	1	4.016547	1.341404	-2.337714
69	1	3.555129	2.543623	-1.128310
70	1	-2.215846	2.818298	3.100861
71	1	-1.591910	1.142953	2.998190
72	1	-3.555179	2.543530	1.128260
73	1	-4.016608	1.341308	2.337659

E(RB3LYP) = -1872.04544128 Hartree
Corrección de punto cero = 0.605894
Suma de las entalpías electrónicas y térmicas = -1871.403703
Suma de las energías libres y térmicas = -1871.503475

[Lu(dpa18c6)]$^{+}$ (vacío) Δ(δλδ)(δλδ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	6	3.519371	-0.748798	-1.098822
2	7	3.019863	-0.410578	0.243211
3	8	1.494249	-1.992278	-1.556371
4	6	2.929807	-2.051207	-1.605276
5	6	3.576328	-1.324058	1.262013
6	6	2.591033	-1.631315	2.367911
7	8	1.410320	-2.208319	1.780220

8	6	0.559544	-2.711599	2.804634
9	6	-0.733883	-3.167758	2.186664
10	8	-1.388215	-2.036350	1.588838
11	8	-1.281750	-2.310886	-1.752593
12	6	-0.404556	-2.830862	-2.745583
13	6	0.905820	-3.187382	-2.097778
14	7	-2.995899	-0.578368	-0.264702
15	6	-3.494403	-1.516280	-1.291818
16	6	-2.473227	-1.792063	-2.373137
17	6	-2.815894	-2.207910	1.585495
18	6	-3.487941	-0.949718	1.070822
19	6	3.309793	0.992198	0.598630
20	6	-3.357252	0.808060	-0.617586
21	6	-2.693500	1.806523	0.301933
22	6	2.588268	1.954589	-0.315428
23	6	-0.892920	2.262276	1.695382
24	6	-1.426544	3.485889	2.086835
25	6	-2.650129	3.873311	1.540453
26	6	-3.301676	3.014814	0.654958
27	6	3.124517	3.195998	-0.669459
28	6	2.421110	4.015384	-1.552389
29	6	1.220634	3.557840	-2.096073
30	6	0.760511	2.304937	-1.704139
31	71	0.015508	-0.433537	-0.001149
32	1	4.393239	1.196889	0.563854
33	1	2.973208	1.159218	1.626708
34	1	-4.450097	0.955875	-0.588301
35	1	-3.025269	0.995044	-1.643810
36	1	-0.886192	4.089029	2.807479
37	1	-3.105164	4.819273	1.819083
38	1	-4.274179	3.269572	0.245448
39	1	4.082227	3.506199	-0.263383
40	1	2.819663	4.986310	-1.831674
41	1	0.644672	4.128793	-2.815346
42	7	1.410289	1.538956	-0.807691
43	7	-1.494792	1.459111	0.797619
44	6	0.395364	1.712238	2.269506
45	8	0.649443	0.495415	1.868853
46	8	1.089029	2.385836	3.018172
47	6	-0.492361	1.676629	-2.276366
48	8	-0.667004	0.444348	-1.879507
49	8	-1.228481	2.306874	-3.022292
50	1	4.620218	-0.829257	-1.130368
51	1	3.243994	-2.203712	-2.646055
52	1	3.268257	-2.917300	-1.023304
53	1	-4.580840	-1.106416	1.087229
54	1	-3.267277	-0.134384	1.762870
55	1	-3.152454	-2.395713	2.613450
56	1	-3.065238	-3.091138	0.984508
57	1	-2.211534	-0.891651	-2.934786
58	1	-2.877231	-2.548737	-3.060262
59	1	-3.748014	-2.465686	-0.814911
60	1	-4.420335	-1.142651	-1.755947
61	1	3.041949	-2.361143	3.054982
62	1	2.302831	-0.736624	2.926204
63	1	4.498922	-0.915012	1.703029
64	1	3.852484	-2.266262	0.783580
65	1	0.777270	-3.928258	-1.297454
66	1	1.569838	-3.612610	-2.859449
67	1	-0.237887	-2.078487	-3.527899

68	1	-0.844126	-3.727703	-3.206942
69	1	3.232735	0.049093	-1.786688
70	1	-1.370645	-3.584259	2.976308
71	1	-0.571562	-3.944451	1.427122
72	1	1.041567	-3.559828	3.313056
73	1	0.360040	-1.924259	3.543324

E(RB3LYP) = -1872.04992593 Hartree
Corrección de punto cero = 0.605557
Suma de las entalpías electrónicas y térmicas = -1871.408151
Suma de las energías libres y térmicas = -1871.509921

[La(dpabp)(H_2O)]$^+$ (vacío) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	6	0	-0.704987	3.530710	-2.522700
2	6	0	-0.369684	2.264939	-2.044010
3	7	0	-0.971678	1.736640	-0.961104
4	6	0	-1.846774	2.467791	-0.257602
5	6	0	-2.228561	3.748222	-0.674096
6	6	0	-1.667963	4.272166	-1.835697
7	6	0	0.706154	1.415982	-2.699880
8	6	0	-2.459162	1.859870	0.997567
9	7	0	1.647552	0.828372	-1.708289
10	7	0	-1.643867	0.836114	1.706761
11	6	0	2.466079	1.850735	-1.000908
12	6	0	-0.700329	1.422298	2.697193
13	6	0	1.856134	2.461892	0.253744
14	6	0	0.378375	2.266447	2.040176
15	6	0	2.243110	3.741125	0.669150
16	6	0	1.684612	4.268345	1.830254
17	6	0	0.718670	3.531292	2.517794
18	7	0	0.978119	1.734718	0.957712
19	1	0	-0.215356	3.932644	-3.403987
20	1	0	-2.944149	4.322995	-0.094081
21	1	0	-1.952619	5.260055	-2.185359
22	1	0	1.243513	2.016937	-3.449475
23	1	0	0.227840	0.579509	-3.224636
24	1	0	-3.395376	1.378204	0.696556
25	1	0	-2.738296	2.668895	1.689273
26	1	0	2.747017	2.658075	-1.693847
27	1	0	3.401153	1.366945	-0.699805
28	1	0	-0.224894	0.584972	3.223169
29	1	0	-1.235675	2.026274	3.445797
30	1	0	2.961042	4.312474	0.088643
31	1	0	1.973221	5.255375	2.179099
32	1	0	0.230640	3.935863	3.398763
33	6	0	2.544899	-0.171959	-2.356872
34	1	0	1.914631	-0.832311	-2.966013
35	1	0	3.260187	0.310524	-3.040202
36	6	0	-2.544108	-0.159519	2.358672
37	1	0	-1.915336	-0.820578	2.968552
38	1	0	-3.256819	0.327224	3.041673
39	6	0	3.281688	-0.990922	-1.306351
40	6	0	4.594854	-1.439761	-1.441455
41	6	0	5.153999	-2.186284	-0.397065
42	1	0	5.169480	-1.212593	-2.334215
43	6	0	3.101791	-1.949206	0.818330

44	6	0	4.406532	-2.442381	0.751723
45	1	0	6.173787	-2.551058	-0.479666
46	1	0	4.797956	-3.002241	1.593318
47	6	0	-3.285099	-0.978445	1.311312
48	6	0	-4.600299	-1.420647	1.448522
49	6	0	-5.163616	-2.167836	0.406864
50	1	0	-5.173292	-1.187880	2.340885
51	6	0	-3.111440	-1.943231	-0.810882
52	6	0	-4.418172	-2.430713	-0.741707
53	1	0	-6.184993	-2.527706	0.491298
54	1	0	-4.812718	-2.991428	-1.581270
55	7	0	2.568660	-1.260012	-0.201612
56	7	0	-2.573964	-1.254104	0.206903
57	6	0	-2.217886	-2.167772	-2.041822
58	8	0	-2.642312	-2.887344	-2.934788
59	8	0	-1.064189	-1.563371	-1.988692
60	6	0	2.206064	-2.167180	2.049012
61	8	0	2.630421	-2.878842	2.948154
62	8	0	1.051206	-1.565236	1.989409
63	57	0	-0.001665	-0.656145	-0.000785
64	8	0	0.008370	-3.338461	-0.018248
65	1	0	0.254132	-3.916946	0.721050
66	1	0	-0.261157	-3.895768	-0.765620

E(RB3LYP) = -1818.94879349 Hartree
Corrección de punto cero = 0.514718
Suma de las entalpías electrónicas y térmicas = -1818.398727
Suma de las energías libres y térmicas = -1818.499827

$[Nd(dpabp)(H_2O)]^+$ (vacío) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	6	0	-0.849872	-3.470020	2.523035
2	6	0	-0.471971	-2.218566	2.039368
3	7	0	-1.011540	-1.703732	0.917231
4	6	0	-1.864508	-2.433103	0.186029
5	6	0	-2.286247	-3.699610	0.606349
6	6	0	-1.789319	-4.210044	1.802373
7	6	0	0.580813	-1.367921	2.728195
8	6	0	-2.403561	-1.837833	-1.108030
9	7	0	1.558464	-0.800047	1.760594
10	7	0	-1.558530	-0.800111	-1.760604
11	6	0	2.403562	-1.837707	1.108008
12	6	0	-0.580870	-1.367910	-2.728230
13	6	0	1.864571	-2.432967	-0.186088
14	6	0	0.472002	-2.218486	-2.039427
15	6	0	2.286414	-3.699424	-0.606453
16	6	0	1.789522	-4.209861	-1.802490
17	6	0	0.850004	-3.469898	-2.523128
18	7	0	1.011543	-1.703646	-0.917273
19	1	0	-0.410655	-3.862645	3.434547
20	1	0	-2.982627	-4.274243	0.003200
21	1	0	-2.105152	-5.187356	2.155013
22	1	0	1.087478	-1.961210	3.504438
23	1	0	0.085743	-0.520591	3.217638
24	1	0	-3.368028	-1.375831	-0.872033
25	1	0	-2.619252	-2.651598	-1.816045

26	1	0	2.619267	-2.651490	1.815997
27	1	0	3.368020	-1.375658	0.872060
28	1	0	-0.085876	-0.520550	-3.217705
29	1	0	-1.087499	-1.961244	-3.504463
30	1	0	2.982841	-4.274021	-0.003327
31	1	0	2.105433	-5.187136	-2.155163
32	1	0	0.410812	-3.862538	-3.434646
33	6	0	2.426615	0.223035	2.412932
34	1	0	1.771216	0.893178	2.982930
35	1	0	3.125989	-0.235332	3.128232
36	6	0	-2.426780	0.222952	-2.412835
37	1	0	-1.771473	0.893148	-2.982879
38	1	0	-3.126200	-0.235423	-3.128086
39	6	0	3.182955	1.018628	1.358910
40	6	0	4.486682	1.490250	1.508060
41	6	0	5.060403	2.207141	0.450893
42	1	0	5.043343	1.302130	2.421029
43	6	0	3.039881	1.904178	-0.800876
44	6	0	4.336962	2.414443	-0.723336
45	1	0	6.073623	2.587417	0.543788
46	1	0	4.741985	2.949107	-1.574863
47	6	0	-3.183049	1.018492	-1.358710
48	6	0	-4.486705	1.490320	-1.507832
49	6	0	-5.060302	2.207247	-0.450623
50	1	0	-5.043397	1.302349	-2.420813
51	6	0	-3.039794	1.903966	0.801092
52	6	0	-4.336798	2.414429	0.723592
53	1	0	-6.073464	2.587682	-0.543486
54	1	0	-4.741709	2.949178	1.575117
55	7	0	2.493692	1.242086	0.229607
56	7	0	-2.493764	1.241764	-0.229397
57	6	0	-2.162696	2.066936	2.052072
58	8	0	-2.599320	2.732064	2.980030
59	8	0	-1.003953	1.471324	1.978191
60	6	0	2.162918	2.067116	-2.051959
61	8	0	2.599702	2.732153	-2.979912
62	8	0	1.004141	1.471596	-1.978143
63	60	0	-0.000015	0.607645	-0.000044
64	8	0	-0.001086	3.243314	-0.000611
65	1	0	0.238824	3.810489	-0.750331
66	1	0	-0.238241	3.811003	0.749595

E(RB3LYP) = -1820.86388839 Hartree
Corrección de punto cero = 0.514910
Suma de las entalpías electrónicas y térmicas = -1820.313739
Suma de las energías libres y térmicas = -1820.413789

[Gd(dpabp)(H_2O)]$^+$ (vacío) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	6	0	-0.966203	3.425870	-2.520616
2	6	0	-0.547193	2.189173	-2.033359
3	7	0	-1.036592	1.681489	-0.884665
4	6	0	-1.880006	2.404690	-0.136211
5	6	0	-2.341013	3.656135	-0.559614
6	6	0	-1.894459	4.158615	-1.778526
7	6	0	0.493555	1.345775	-2.746992

8	6	0	-2.360368	1.818393	1.184124
9	7	0	1.487489	0.778965	-1.797008
10	7	0	-1.487052	0.779661	1.796882
11	6	0	2.361252	1.817349	-1.184318
12	6	0	-0.492869	1.346088	2.746834
13	6	0	1.881273	2.403765	0.136098
14	6	0	0.548329	2.188914	2.033210
15	6	0	2.343057	3.654888	0.559611
16	6	0	1.896805	4.157550	1.778555
17	6	0	0.968084	3.425318	2.520566
18	7	0	1.037415	1.681009	0.884480
19	1	0	-0.566332	3.813159	-3.452282
20	1	0	-3.028265	4.225455	0.058873
21	1	0	-2.240673	5.124670	-2.133663
22	1	0	0.984764	1.943223	-3.529649
23	1	0	-0.009157	0.497901	-3.225645
24	1	0	-3.339006	1.363118	0.998437
25	1	0	-2.535683	2.635947	1.898427
26	1	0	2.536754	2.634874	-1.898607
27	1	0	3.339761	1.361735	-0.998785
28	1	0	0.009399	0.498004	3.225580
29	1	0	-0.983825	1.943835	3.529421
30	1	0	3.030671	4.223826	-0.058826
31	1	0	2.243615	5.123360	2.133776
32	1	0	0.568439	3.812778	3.452259
33	6	0	2.324502	-0.267733	-2.451427
34	1	0	1.644847	-0.938438	-2.990604
35	1	0	3.016148	0.165867	-3.189072
36	6	0	-2.324500	-0.266563	2.451517
37	1	0	-1.645086	-0.937487	2.990720
38	1	0	-3.015880	0.167473	3.189155
39	6	0	3.086331	-1.051309	-1.393716
40	6	0	4.376178	-1.557604	-1.551025
41	6	0	4.952557	-2.255601	-0.482951
42	1	0	4.920238	-1.409357	-2.478785
43	6	0	2.960568	-1.874834	0.791541
44	6	0	4.244956	-2.413963	0.708876
45	1	0	5.955604	-2.660610	-0.581491
46	1	0	4.653160	-2.933184	1.568435
47	6	0	-3.086792	-1.049948	1.394016
48	6	0	-4.376931	-1.555456	1.551462
49	6	0	-4.953781	-2.253287	0.483532
50	1	0	-4.920864	-1.406722	2.479218
51	6	0	-2.961684	-1.873782	-0.791168
52	6	0	-4.246358	-2.412206	-0.708328
53	1	0	-5.957058	-2.657697	0.582196
54	1	0	-4.654924	-2.931291	-1.567797
55	7	0	2.412900	-1.227246	-0.247099
56	7	0	-2.413515	-1.226464	0.247386
57	6	0	-2.093932	-1.986837	-2.051687
58	8	0	-2.528701	-2.620556	-3.001851
59	8	0	-0.937941	-1.385879	-1.961823
60	6	0	2.092613	-1.987420	2.051944
61	8	0	2.527272	-2.620571	3.002523
62	8	0	0.936532	-1.386628	1.961614
63	64	0	-0.000178	-0.551989	-0.000144
64	8	0	0.000352	-3.147813	-0.000834
65	1	0	0.203695	-3.714741	0.759511
66	1	0	-0.207381	-3.714583	-0.760114

E(RB3LYP) = -1823.28054306 Hartree
Corrección de punto cero = 0.515471
Suma de las entalpías electrónicas y térmicas = -1822.730037
Suma de las energías libres y térmicas = -1822.829005

[Ho(dpabp)(H_2O)]$^+$ (vacío) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	6	0	1.024442	-3.405998	-2.516362
2	6	0	0.582594	-2.177682	-2.028303
3	7	0	1.047559	-1.670692	-0.868852
4	6	0	1.890020	-2.388368	-0.113533
5	6	0	2.373135	-3.630958	-0.537492
6	6	0	1.950676	-4.131920	-1.765477
7	6	0	-0.455427	-1.342725	-2.753951
8	6	0	2.342829	-1.804400	1.216637
9	7	0	-1.452071	-0.770413	-1.811856
10	7	0	1.451849	-0.770747	1.811803
11	6	0	-2.343277	-1.803881	-1.216712
12	6	0	0.455071	-1.342853	2.753883
13	6	0	-1.890653	-2.387901	0.113492
14	6	0	-0.583166	-2.177535	2.028244
15	6	0	-2.374137	-3.630333	0.537499
16	6	0	-1.951823	-4.131381	1.765497
17	6	0	-1.025366	-3.405706	2.516347
18	7	0	-1.047982	-1.670440	0.868781
19	1	0	0.642867	-3.792172	-3.456115
20	1	0	3.058689	-4.194739	0.087904
21	1	0	2.313857	-5.091530	-2.121123
22	1	0	-0.942885	-1.947342	-3.533311
23	1	0	0.048083	-0.497882	-3.235634
24	1	0	3.323862	-1.346162	1.051976
25	1	0	2.506131	-2.622850	1.932526
26	1	0	-2.506684	-2.622319	-1.932590
27	1	0	-3.324236	-1.345462	-1.052122
28	1	0	-0.048222	-0.497897	3.235595
29	1	0	0.942395	-1.947604	3.533223
30	1	0	-3.059862	-4.193928	-0.087877
31	1	0	-2.315289	-5.090869	2.121179
32	1	0	-0.643898	-3.791960	3.456111
33	6	0	-2.270069	0.289498	-2.467804
34	1	0	-1.576345	0.956890	-2.992137
35	1	0	-2.960179	-0.130121	-3.214788
36	6	0	2.270061	0.288931	2.467862
37	1	0	1.576453	0.956432	2.992207
38	1	0	2.960043	-0.130903	3.214843
39	6	0	-3.029643	1.070289	-1.407977
40	6	0	-4.310024	1.599812	-1.567061
41	6	0	-4.883896	2.289907	-0.492779
42	1	0	-4.848647	1.474475	-2.501324
43	6	0	-2.907065	1.860886	0.788889
44	6	0	-4.182472	2.419717	0.706356
45	1	0	-5.879928	2.711633	-0.592278
46	1	0	-4.589002	2.932181	1.570764
47	6	0	3.029866	1.069632	1.408145
48	6	0	4.310414	1.598734	1.567293
49	6	0	4.884535	2.288732	0.493082

50	1	0	4.848983	1.473135	2.501552
51	6	0	2.907630	1.860366	-0.788695
52	6	0	4.183198	2.418825	-0.706074
53	1	0	5.880697	2.710136	0.592640
54	1	0	4.589922	2.931199	-1.570444
55	7	0	-2.362120	1.218490	-0.254342
56	7	0	2.362409	1.218141	0.254504
57	6	0	2.041920	1.943963	-2.050452
58	8	0	2.471237	2.558888	-3.015007
59	8	0	0.888618	1.338442	-1.946434
60	6	0	-2.041239	1.944275	2.050567
61	8	0	-2.470509	2.558871	3.015344
62	8	0	-0.887857	1.338900	1.946291
63	67	0	0.000074	0.516625	-0.000081
64	8	0	-0.000361	3.101594	-0.000475
65	1	0	-0.177802	3.669138	0.765896
66	1	0	0.180713	3.669180	-0.765967

E(RB3LYP) = -1825.04617687 Hartree
Corrección de punto cero= 0.515817 (/Particle)
Suma de las entalpías electrónicas y térmicas= -1824.495396
Suma de las energías libres y térmicas= -1824.594158

[Yb(dpabp)(H_2O)]$^+$ (vacío) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	6	0	-1.049190	3.398471	-2.512793
2	6	0	-0.595780	2.174282	-2.025015
3	7	0	-1.047602	1.667247	-0.860033
4	6	0	-1.889258	2.382826	-0.101203
5	6	0	-2.383266	3.620986	-0.524688
6	6	0	-1.973552	4.121379	-1.757140
7	6	0	0.440259	1.344701	-2.758307
8	6	0	-2.328274	1.799996	1.233286
9	7	0	1.433113	0.762465	-1.820118
10	7	0	-1.426966	0.770348	1.818853
11	6	0	2.340437	1.786758	-1.234539
12	6	0	-0.430185	1.346416	2.756800
13	6	0	1.906339	2.370262	0.101053
14	6	0	0.611312	2.169248	2.024237
15	6	0	2.410191	3.603818	0.526472
16	6	0	2.004370	4.105775	1.759522
17	6	0	1.074078	3.389156	2.513872
18	7	0	1.059060	1.660068	0.858701
19	1	0	-0.676930	3.783806	-3.456614
20	1	0	-3.067338	4.181859	0.104917
21	1	0	-2.344997	5.077911	-2.112525
22	1	0	0.929669	1.955662	-3.531369
23	1	0	-0.064710	0.505581	-3.247252
24	1	0	-3.309606	1.338826	1.078581
25	1	0	-2.487272	2.618672	1.949741
26	1	0	2.502378	2.605421	-1.950317
27	1	0	3.319636	1.320520	-1.081766
28	1	0	0.069192	0.503868	3.245603
29	1	0	-0.915823	1.960238	3.529985
30	1	0	3.098873	4.159984	-0.102280
31	1	0	2.383473	5.058742	2.116382

32	1	0	0.704701	3.775969	3.458216
33	6	0	2.234711	-0.309884	-2.474769
34	1	0	1.530572	-0.970378	-2.993139
35	1	0	2.929985	0.097320	-3.223714
36	6	0	-2.233906	-0.295856	2.476711
37	1	0	-1.532446	-0.959051	2.995122
38	1	0	-2.925730	0.116890	3.225828
39	6	0	2.982180	-1.093848	-1.409986
40	6	0	4.250687	-1.652341	-1.565957
41	6	0	4.813113	-2.341215	-0.485181
42	1	0	4.788711	-1.549398	-2.503282
43	6	0	2.847517	-1.859642	0.793920
44	6	0	4.111342	-2.443566	0.716592
45	1	0	5.800082	-2.784354	-0.581784
46	1	0	4.508919	-2.955017	1.585749
47	6	0	-2.988017	-1.077525	1.415300
48	6	0	-4.262502	-1.622053	1.572571
49	6	0	-4.832926	-2.307148	0.493550
50	1	0	-4.799365	-1.510636	2.509591
51	6	0	-2.864131	-1.846178	-0.788518
52	6	0	-4.133563	-2.417891	-0.708934
53	1	0	-5.824527	-2.739505	0.591599
54	1	0	-4.537621	-2.925149	-1.577591
55	7	0	2.314333	-1.214809	-0.253787
56	7	0	-2.321475	-1.208471	0.259066
57	6	0	-1.997366	-1.907789	-2.048933
58	8	0	-2.416607	-2.516595	-3.021798
59	8	0	-0.851101	-1.291312	-1.934151
60	6	0	1.976764	-1.917117	2.050955
61	8	0	2.394011	-2.515452	3.030738
62	8	0	0.826831	-1.306460	1.928265
63	70	0	-0.001183	-0.485233	-0.003063
64	8	0	0.024219	-3.073156	-0.013683
65	1	0	0.079383	-3.627385	0.780525
66	1	0	-0.216747	-3.640352	-0.762840

E(RB3LYP) = -1826.79723890 Hartree
Corrección de punto cero = 0.516157
Suma de las entalpías electrónicas y térmicas = -1826.246218
Suma de las energías libres y térmicas = -1826.344568

(1) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.503278
3	8	2.387770	0.000000	0.669864
4	8	-1.675024	1.681239	0.771716
5	8	-1.350111	0.635132	-2.008098
6	8	-2.161566	-1.215357	0.227490
7	8	0.520283	-2.377358	0.669270
8	8	0.968523	-1.216366	-1.953911
9	1	2.925806	-0.711301	1.073983
10	1	3.009608	0.733248	0.484398
11	1	0.767107	0.240012	3.063145
12	1	-0.710224	-0.239675	3.133868
13	1	-1.854095	2.011900	1.674895
14	1	-2.162928	2.284457	0.175352

15	1	0.758350	-3.119810	0.078343
16	1	0.486264	-2.764311	1.567334
17	1	-2.294912	-2.184570	0.262610
18	1	-3.045829	-0.825167	0.382821
19	1	-2.177688	0.243572	-2.355510
20	1	-1.125069	1.364447	-2.621360
21	1	1.882518	-1.546886	-2.073910
22	1	0.526321	-1.365904	-2.814624
23	7	1.081242	2.130403	-0.859283
24	6	1.716348	2.171069	-2.065317
25	6	1.078630	3.271728	-0.114814
26	6	2.340924	3.316776	-2.552818
27	1	1.726425	1.248512	-2.640669
28	6	1.690298	4.450760	-0.535399
29	1	0.565604	3.230480	0.842944
30	6	2.329703	4.480131	-1.777801
31	1	2.829343	3.293070	-3.523238
32	1	1.659957	5.330410	0.101786
33	1	2.810785	5.388183	-2.132952

HF = -813.1053412
Corrección de punto cero = 0.266299 (Hartree/Particle)
Suma de las entalpías electrónicas y térmicas = -815.081202
Suma de las energías libres y térmicas = -815.163231

(2) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.215201
3	8	2.494850	0.000000	-0.269634
4	8	0.970392	2.092719	1.002280
5	8	0.681527	1.159577	-2.165070
6	8	-1.876548	1.579074	-0.490447
7	8	-2.277853	-0.892705	0.709245
8	8	-0.531444	-1.546345	-1.896005
9	1	3.079420	-0.779719	-0.203175
10	1	2.938487	0.710960	0.235066
11	1	0.800924	1.923981	1.957018
12	1	1.085364	3.054344	0.888220
13	1	-2.899502	-1.584682	0.413602
14	1	-2.350543	-0.863713	1.685455
15	1	-2.760573	1.272347	-0.209527
16	1	-1.934089	2.551275	-0.550840
17	1	0.220425	1.775775	-2.765092
18	1	1.624202	1.187886	-2.419207
19	1	-0.846523	-2.470235	-1.902723
20	1	-0.485339	-1.271003	-2.831940
21	6	0.233061	-1.030883	3.037432
22	8	0.085986	-1.026179	4.247856
23	7	0.748925	-2.250004	0.960739
24	6	0.709217	-2.278158	2.321185
25	6	1.189650	-3.359139	0.316421
26	6	1.090239	-3.401255	3.058995
27	6	1.595219	-4.511405	0.987147
28	6	1.540614	-4.535674	2.384036
29	1	1.026214	-3.355822	4.142519
30	1	1.847144	-5.421593	2.934076

31	1	1.944754	-5.371181	0.422731
32	1	1.224775	-3.307454	-0.770047

HF = -924.5286309
Corrección de punto cero = 0.242913 (Hartree/Particle)
Suma de las entalpías electrónicas y térmicas = -926.826773
Suma de las energías libres y térmicas = -926.909234

(3) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	7	0.000000	0.000000	2.530074
3	7	2.284357	0.000000	1.052397
4	8	1.150653	1.862362	-1.257811
5	8	-1.024102	2.143929	0.718878
6	8	-1.297726	0.611110	-2.089648
7	8	-2.329549	-0.897329	0.193330
8	8	0.058786	-2.413001	0.681489
9	8	1.010917	-1.270428	-1.902479
10	1	1.771308	1.808694	-2.012003
11	1	1.343377	2.725066	-0.837289
12	1	-1.080176	2.442519	1.649271
13	1	-1.511850	2.814180	0.197748
14	1	0.161747	-3.231689	0.155486
15	1	0.219183	-2.676394	1.610045
16	1	-2.508024	-1.822361	0.457066
17	1	-3.206677	-0.468999	0.125955
18	1	-2.123252	0.228494	-2.448410
19	1	-1.079872	1.360332	-2.679067
20	1	1.768170	-1.889915	-1.926929
21	1	0.641060	-1.278635	-2.808712
22	6	2.423031	-0.038698	2.410513
23	6	1.182309	0.093876	3.210197
24	6	3.401061	-0.096227	0.286726
25	6	-1.160603	0.064736	3.236299
26	6	3.683321	-0.205189	3.002506
27	6	1.200513	0.298933	4.597842
28	6	0.002362	0.368515	5.308834
29	6	4.681382	-0.239039	0.814855
30	6	-1.204120	0.236039	4.617595
31	6	4.822111	-0.301148	2.202506
32	1	3.254739	-0.047154	-0.789728
33	1	5.541883	-0.304972	0.154796
34	1	5.801963	-0.425847	2.657023
35	1	3.788312	-0.273607	4.080298
36	1	2.138390	0.419185	5.130132
37	1	0.012512	0.523822	6.385031
38	1	-2.159725	0.271396	5.133637
39	1	-2.077335	-0.039690	2.661640

HF = -982.6591289 Hartree
Corrección de punto cero = 0.310419
Suma de las entalpías electrónicas y térmicas = -985.189503
Suma de las energías libres y térmicas = -985.275583

(4) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.452713
3	8	2.231681	0.000000	0.971247
4	8	1.169620	1.816004	-1.287078
5	8	-1.076308	2.155702	0.611465
6	8	-1.294399	0.503236	-2.093222
7	8	-2.357044	-0.785508	0.270757
8	8	-0.010517	-2.426069	0.611563
9	8	1.064351	-1.267837	-1.869423
10	1	1.790302	1.739305	-2.039967
11	1	1.299887	2.725691	-0.948321
12	1	-1.155973	2.560139	1.499364
13	1	-1.563043	2.760845	0.014039
14	1	0.119695	-3.206965	0.035429
15	1	-0.020575	-2.776740	1.525306
16	1	-2.608810	-1.716228	0.439917
17	1	-3.195357	-0.280337	0.300647
18	1	-2.145222	0.114386	-2.381458
19	1	-1.076091	1.180546	-2.765025
20	1	1.870021	-1.824051	-1.892000
21	1	0.689567	-1.325070	-2.772470
22	6	2.374170	-0.338054	2.386426
23	6	1.255022	0.334658	3.130658
24	1	3.336744	0.035181	2.750399
25	1	2.350961	-1.427561	2.491407
26	1	1.216559	-0.032472	4.161171
27	1	1.368566	1.424139	3.141959
28	6	3.525156	-0.098262	0.282324
29	1	4.203246	0.651346	0.692513
30	1	3.342823	0.101766	-0.770980
31	1	3.934130	-1.101444	0.422151
32	6	-1.138205	0.123910	3.375510
33	1	-1.030631	-0.614090	4.172031
34	1	-2.037444	-0.072538	2.797210
35	1	-1.157453	1.130011	3.801537

HF = -797.354464 Hartree
Corrección de punto cero = 0.297762
Suma de las entalpías electrónicas y térmicas = -799.198386
Suma de las energías libres y térmicas = -799.279720

(5) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	7	0.000000	0.000000	2.660159
3	7	2.449754	0.000000	0.902083
4	8	0.961993	1.795279	-1.473388
5	8	-1.229591	2.136173	0.387330
6	8	-1.433377	0.233865	-2.084009
7	8	-2.398702	-0.721718	0.420726
8	8	-0.061925	-2.484355	0.205411
9	8	1.097860	-1.128883	-1.994272

10	1	1.568813	1.642644	-2.225534
11	1	1.018071	2.755372	-1.290136
12	1	-1.427311	2.618446	1.215578
13	1	-1.689931	2.635986	-0.318007
14	1	0.225779	-3.069735	-0.524365
15	1	-0.295392	-3.083093	0.943452
16	1	-2.759549	-1.630915	0.439540
17	1	-3.153328	-0.142660	0.650434
18	1	-2.325987	-0.151487	-2.190630
19	1	-1.300202	0.807409	-2.865011
20	1	1.994331	-1.498648	-2.123262
21	1	0.631858	-1.266004	-2.843794
22	6	2.409303	-0.548795	2.294110
23	6	1.400792	0.168564	3.165936
24	1	3.406081	-0.462505	2.750177
25	1	2.186924	-1.619369	2.228787
26	1	1.470072	-0.209721	4.195175
27	1	1.624589	1.237200	3.216447
28	6	2.996599	1.391073	0.947758
29	6	3.427518	-0.830193	0.139643
30	1	3.082769	-1.866972	0.096702
31	1	3.552190	-0.422346	-0.866363
32	1	4.409580	-0.817921	0.626748
33	1	3.899527	1.429350	1.568845
34	1	3.261291	1.708791	-0.060419
35	1	2.266102	2.092942	1.358594
36	6	-0.837529	1.055734	3.301789
37	6	-0.513575	-1.309669	3.166422
38	1	-0.570272	-1.298863	4.261029
39	1	-1.514839	-1.492541	2.773547
40	1	0.162452	-2.116902	2.879997
41	1	-0.788667	0.977999	4.394123
42	1	-0.462552	2.045480	3.027323
43	1	-1.881424	0.937701	3.000942

HF = -835.7523333 Hartree
Corrección de punto cero = 0.382764
Suma de las entalpías electrónicas y térmicas = -837.762735
Suma de las energías libres y térmicas = -837.846252

(6) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	7	0.000000	0.000000	2.620026
3	8	2.253377	0.000000	0.939195
4	8	1.039358	1.977726	-1.136601
5	8	-1.418993	2.016756	0.411231
6	8	-1.313047	0.444589	-2.129264
7	8	-2.317291	-0.897357	0.295002
8	8	0.033213	-2.508644	0.111222
9	8	1.186661	-1.011354	-1.997276
10	1	1.838071	1.994366	-1.702265
11	1	0.906654	2.908326	-0.862638
12	1	-1.669398	2.488844	1.230671
13	1	-1.928991	2.452233	-0.302053
14	1	0.294378	-3.069342	-0.646954
15	1	-0.055063	-3.123408	0.867491

16	1	-2.573939	-1.840483	0.249333
17	1	-3.138330	-0.414248	0.518658
18	1	-2.160136	0.028384	-2.388708
19	1	-1.111957	1.090162	-2.836857
20	1	2.029264	-1.497085	-2.107410
21	1	0.803055	-0.959945	-2.896122
22	6	2.483485	0.031246	2.387394
23	6	1.274377	0.655481	3.037215
24	1	3.363275	0.650790	2.586660
25	1	2.694021	-0.986729	2.727046
26	1	1.389904	0.611112	4.130440
27	1	1.219402	1.714747	2.759053
28	6	3.531522	-0.154926	0.236958
29	1	3.986599	-1.107977	0.515010
30	1	3.321228	-0.125142	-0.829809
31	1	4.189812	0.673198	0.504817
32	6	-1.114253	0.722591	3.302600
33	6	-0.027227	-1.402532	3.130353
34	1	0.116884	-1.420854	4.217341
35	1	-1.003026	-1.843380	2.911655
36	1	0.765851	-1.996903	2.673320
37	1	-1.058284	0.579058	4.387618
38	1	-1.033405	1.795073	3.112572
39	1	-2.075454	0.341555	2.952848

HF = -816.5538526 Hartree
Corrección de punto cero = 0.340197
Suma de las entalpías electrónicas y térmicas = -818.480651
Suma de las energías libres y térmicas = -818.564366

(7) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.231236
3	7	2.416073	0.000000	1.022372
4	8	0.575526	2.077819	-1.257419
5	8	-1.105883	2.039298	0.970991
6	8	-1.636214	-0.075449	-1.950524
7	8	-2.063375	-1.056793	1.059238
8	8	-0.020815	-2.476769	-0.059481
9	8	1.344102	-0.666772	-2.054386
10	1	1.144485	2.199497	-2.040959
11	1	0.442369	2.963513	-0.867129
12	1	-1.009106	1.852472	1.931898
13	1	-1.872778	2.634322	0.868276
14	1	0.542338	-3.194469	-0.404997
15	1	-0.708663	-2.895130	0.496088
16	1	-3.037570	-1.060490	1.007249
17	1	-1.819667	-0.877372	1.997204
18	1	-2.319897	-0.750689	-2.126455
19	1	-1.869546	0.682538	-2.520892
20	1	2.289650	-0.883998	-2.157473
21	1	0.911894	-0.951674	-2.882418
22	6	2.278370	-0.740169	2.308232
23	6	1.010554	-0.337291	3.062047
24	6	2.751743	1.415135	1.343943
25	6	3.551533	-0.580676	0.266207

26	1	3.328911	-1.617817	0.000063
27	1	3.733423	0.013008	-0.634458
28	1	4.470769	-0.570870	0.863995
29	1	3.680350	1.469737	1.925062
30	1	2.884988	1.980345	0.418784
31	1	1.950093	1.863556	1.935807
32	8	0.935095	-0.372585	4.272273
33	1	3.151746	-0.578864	2.952493
34	1	2.218303	-1.813984	2.090666

HF = -851.0805349 Hartree
Corrección de punto cero = 0.278606
Suma de las entalpías electrónicas y térmicas = -853.120092
Suma de las energías libres y térmicas = -853.200882

(8) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.528203
3	7	2.641575	0.000000	0.409850
4	8	0.237830	2.478262	0.272869
5	8	-2.434505	0.478054	0.500118
6	8	-1.534743	0.307279	-2.040487
7	8	-0.691162	-2.253648	0.706491
8	8	0.887689	-3.784732	-0.686454
9	15	1.930718	-0.113920	-2.210523
10	1	0.687745	2.555174	-0.607981
11	1	-0.252342	3.301593	0.440708
12	1	0.328150	0.651268	3.174262
13	1	-0.053664	-0.855466	2.993741
14	1	-2.989858	0.773762	1.242086
15	1	-2.895638	0.708339	-0.330156
16	1	1.112995	-3.032720	-1.295107
17	1	0.722623	-4.567979	-1.237359
18	1	-0.181374	-2.989035	0.219660
19	1	-1.581309	-2.597035	0.897030
20	1	-1.695873	-0.451714	-2.633166
21	1	-0.755976	0.778011	-2.446379
22	6	3.260258	0.084853	-0.958322
23	1	4.049244	-0.667243	-1.074126
24	1	3.718977	1.068609	-1.093835
25	6	2.963784	-1.315864	1.009720
26	6	3.193130	1.063142	1.274966
27	8	1.067635	-1.302856	-1.539889
28	8	0.988086	1.132090	-1.796518
29	8	2.376374	-0.254321	-3.621247
30	1	2.488447	-1.393920	1.992485
31	1	4.047727	-1.432746	1.141741
32	1	2.596055	-2.113365	0.363715
33	1	2.762370	0.975777	2.276672
34	1	2.937446	2.040153	0.862480
35	1	4.284611	0.980971	1.359487

HF = -1229.1599671 Hartree
Corrección de punto cero = 0.279579
Suma de las entalpías electrónicas y térmicas = -1231.395390
Suma de las energías libres y térmicas = -1231.477132

(9) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.344026
3	7	2.388184	0.000000	1.111013
4	8	0.769262	1.907113	-1.410250
5	8	-1.015206	2.157417	0.757145
6	8	-1.540524	-0.149983	-2.010427
7	8	-2.197102	-0.791485	0.913910
8	8	-0.047063	-2.472898	0.090957
9	8	1.346342	-0.896113	-1.958452
10	1	1.282888	1.849288	-2.240610
11	1	0.734854	2.858575	-1.184398
12	1	-1.096651	2.287814	1.723490
13	1	-1.638450	2.796009	0.354514
14	1	0.477994	-3.144156	-0.388404
15	1	-0.735457	-2.967396	0.580095
16	1	-3.116469	-0.797820	0.580783
17	1	-2.263075	-0.748061	1.888763
18	1	-2.167056	-0.861569	-2.254383
19	1	-1.724825	0.570891	-2.646840
20	1	2.293679	-1.110384	-2.067147
21	1	0.921183	-1.168205	-2.796462
22	6	2.289740	-0.720407	2.407088
23	6	0.989313	-0.358632	3.102410
24	6	2.714217	1.429444	1.399154
25	6	3.532379	-0.584480	0.356779
26	1	3.323508	-1.629835	0.114643
27	1	3.695406	-0.004411	-0.554701
28	1	4.456597	-0.544410	0.945139
29	1	3.651738	1.507936	1.963059
30	1	2.834016	1.970891	0.459290
31	1	1.914614	1.890024	1.985186
32	7	0.881923	-0.444356	4.410384
33	6	1.979394	-0.903709	5.293910
34	6	-0.362331	-0.069370	5.107942
35	1	-0.100272	0.588892	5.938475
36	1	-1.026642	0.447390	4.421006
37	1	-0.840645	-0.971032	5.497477
38	1	1.522126	-1.369394	6.167118
39	1	2.597918	-1.649141	4.797766
40	1	2.581377	-0.050426	5.616147
41	1	3.166462	-0.490482	3.024680
42	1	2.295054	-1.802283	2.216794

HF = -909.5236711 Hartree
Corrección de punto cero = 0.362054
Suma de las entalpías electrónicas y térmicas = -911.710278
Suma de las energías libres y térmicas = -911.798818

(10) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.456708

3	8	2.025783	0.000000	0.893557
4	8	1.459042	1.730498	-1.060148
5	8	-1.101521	2.141317	0.742162
6	8	-1.000693	0.315810	-2.281774
7	8	-2.467983	-0.393879	0.359112
8	8	-0.377835	-2.444659	0.241352
9	8	1.608249	-1.446526	-1.338071
10	1	2.305070	1.668665	-0.566964
11	1	1.527084	2.499687	-1.655555
12	1	-0.887270	2.463674	1.639657
13	1	-1.292415	2.942858	0.217108
14	1	0.283082	-2.964626	-0.259150
15	1	-0.693177	-3.020582	0.963508
16	1	-2.986776	-1.218800	0.300950
17	1	-3.093458	0.304062	0.633237
18	1	-1.914929	0.093806	-2.544395
19	1	-0.548211	0.576961	-3.106900
20	1	2.442518	-1.298264	-0.839601
21	1	1.859011	-1.624942	-2.264211
22	6	2.416509	-0.161874	2.166817
23	6	1.284846	-0.087868	3.198139
24	1	-0.719857	-0.156695	3.099659
25	8	3.558130	-0.347324	2.539014
26	6	1.288328	-1.280507	4.130278
27	1	1.394142	0.847114	3.758663
28	1	0.510167	-1.196601	4.895210
29	1	1.152947	-2.210989	3.571335
30	1	2.257232	-1.322543	4.632776

HF = -831.8961321 Hartree
Corrección de punto cero = 0.235430
Suma de las entalpías electrónicas y térmicas = -833.855628
Suma de las energías libres y térmicas = -833.936280

(11) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.549854
3	8	2.003993	0.000000	0.988846
4	8	0.937040	1.767228	-1.586496
5	8	-1.089905	2.029451	0.976201
6	8	-1.028153	0.053570	-2.303512
7	8	-2.235102	-1.114456	0.436640
8	8	0.232430	-2.466486	-0.413378
9	8	1.922302	-0.606152	-1.162572
10	1	1.669369	1.104121	-1.744009
11	1	1.364285	2.630387	-1.438492
12	1	0.986898	-0.082901	2.578519
13	1	-0.363212	-0.543914	3.270592
14	1	-0.923627	2.062397	1.938842
15	1	-1.315349	2.932323	0.689012
16	1	1.076863	-2.260593	-0.903285
17	1	0.415557	-3.249921	0.136430
18	1	-2.395271	-2.033305	0.154387
19	1	-3.109952	-0.720403	0.605143
20	1	-1.280881	-0.673439	-2.900763
21	1	-0.542146	0.706635	-2.845254

22	6	2.740057	-0.476680	-0.057489
23	8	3.917230	-0.759727	-0.025889

HF = -753.5310087 Hartree
Corrección de punto cero = 0.166378
Suma de las entalpías electrónicas y térmicas = -755.319896
Suma de las energías libres y térmicas = -755.391618

(12) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.496823
3	8	2.228191	0.000000	0.853267
4	8	0.977697	1.727722	-1.509618
5	8	-0.630090	2.281427	0.804875
6	8	-0.491301	-0.654726	-2.351961
7	8	-2.496477	-0.022110	0.144796
8	8	-0.439031	-2.406319	0.404495
9	8	1.757534	-1.344447	-0.864181
10	1	0.964221	1.630573	-2.481766
11	1	1.786342	2.238072	-1.304911
12	1	0.918278	-0.076038	2.830366
13	1	-0.586593	-0.271170	3.228365
14	1	-0.617919	2.532979	1.748752
15	1	-0.585905	3.115421	0.298205
16	1	0.271664	-2.961775	0.022033
17	1	-0.965131	-2.986768	0.986480
18	1	-3.128155	-0.739145	-0.059116
19	1	-3.042813	0.750298	0.390310
20	1	-1.269684	-0.741256	-2.934887
21	1	0.202019	-1.240319	-2.721884
22	6	2.603411	-0.870154	-0.024340
23	8	3.848351	-1.295157	-0.089812
24	1	4.382687	-0.854477	0.605103

HF = 753.8631207 Hartree
Corrección de punto cero = 0.178580
Suma de las entalpías electrónicas y térmicas = -755.611893
Suma de las energías libres y térmicas = -755.685205

(13) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.570145
3	8	2.064881	0.000000	0.972777
4	8	0.622809	1.618851	-1.770766
5	8	-0.645379	2.169929	1.097774
6	8	-0.665458	-1.357937	-2.008442
7	8	-2.513927	-0.011007	0.246128
8	8	0.169052	-2.373624	0.698896
9	8	1.809113	-0.680224	-1.352552
10	1	1.429280	1.106770	-2.031495
11	1	0.668315	2.503540	-2.171586

12	1	0.984811	-0.119875	2.529921
13	1	-0.340569	-0.750720	3.091414
14	1	-0.495928	2.010262	2.053212
15	1	-0.321676	3.069618	0.910108
16	1	1.166939	-2.593498	0.685525
17	1	-0.259387	-3.097575	0.206226
18	1	-3.180378	-0.687739	0.027876
19	1	-2.993197	0.723250	0.672850
20	1	0.282245	-1.505499	-2.255334
21	1	-1.151968	-1.183935	-2.833831
22	15	2.765714	-0.946940	-0.105118
23	8	2.819540	-2.392054	0.341804
24	8	4.209012	-0.336247	-0.479137
25	1	4.920017	-0.956924	-0.229373

HF = -1131.9472578 Hartree
Corrección de punto cero = 0.178623
Suma de las entalpías electrónicas y térmicas = -1133.896769
Suma de las energías libres y térmicas = -1133.969994

(14) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.490926
3	8	2.332558	0.000000	1.010631
4	8	0.719131	2.365567	-0.431830
5	8	-1.844911	1.572971	0.786861
6	8	-1.733735	0.122105	-1.805366
7	8	-1.827225	-1.685212	0.405136
8	9	0.730085	-1.957940	-0.175433
9	8	1.364586	-0.168650	-2.093292
10	1	1.511466	2.749583	-0.852861
11	1	0.179876	3.124111	-0.136438
12	1	2.712966	-0.893047	0.882158
13	1	3.089641	0.612520	1.069214
14	1	0.894387	-0.039825	2.882705
15	1	-0.599248	-0.418846	3.137174
16	1	-2.021918	1.895772	1.690618
17	1	-2.637366	1.791846	0.260582
18	1	-1.362028	-2.546879	0.361485
19	1	-2.687995	-1.844222	0.834426
20	1	-2.332854	-0.648003	-1.858797
21	1	-1.664033	0.471421	-2.714315
22	1	1.641798	-1.104100	-2.174042
23	1	1.676729	0.287646	-2.896076

HF = -666.2672256 Hartree
Corrección de punto cero = 0.175824
Suma de las entalpías electrónicas y térmicas = -667.737358
Suma de las energías libres y térmicas = -667.811096

(15) MP2/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.487550
3	8	2.376711	0.000000	0.734860
4	8	1.083643	1.994692	-1.017779
5	8	-1.294774	1.993389	0.733953
6	8	-1.456953	0.413990	-1.973785
7	8	-2.221736	-0.998697	0.504730
8	8	0.373999	-2.407268	0.504405
9	8	1.137255	-0.997471	-1.975064
10	1	1.726838	2.029524	-1.756187
11	1	0.928331	2.930090	-0.770755
12	1	2.893075	-0.733010	1.130094
13	1	3.008378	0.745311	0.659943
14	1	0.765939	0.188225	3.068944
15	1	-0.737983	-0.208347	3.097576
16	1	-1.316281	2.372400	1.637277
17	1	-1.905605	2.551313	0.208841
18	1	0.624750	-3.103738	-0.137582
19	1	0.332274	-2.862530	1.371094
20	1	-2.430865	-1.954619	0.555546
21	1	-3.061792	-0.542211	0.719391
22	1	-2.318477	-0.013804	-2.160514
23	1	-1.319962	1.043957	-2.711704
24	1	2.071082	-1.280836	-2.063560
25	1	0.735820	-1.164915	-2.853081

HF = -642.3941312 Hartree
Corrección de punto cero = 0.200557
Suma de las entalpías electrónicas y térmicas = -643.837429
Suma de las energías libres y térmicas = -643.909957

(16) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	-0.012507	0.000718	-0.522053
2	8	-1.014902	-2.084576	-1.256537
3	8	-2.136884	0.998018	-1.161769
4	8	1.021948	2.052411	-1.279421
5	8	2.101768	-1.002417	-1.219021
6	8	-0.086670	-0.033039	-2.995249
7	1	0.428146	0.556528	-3.584000
8	1	-0.283081	-0.843076	-3.509943
9	7	-1.927322	-0.936579	1.126097
10	7	-0.913207	1.948548	1.116556
11	7	1.945425	0.937276	1.109981
12	7	0.933000	-1.936122	1.116627
13	7	-2.718272	-3.595088	-1.304679
14	1	-2.314682	-4.080536	-2.109179
15	1	-3.614045	-3.938626	-0.955112
16	7	-3.596601	2.740675	-1.289144
17	1	-4.089357	2.316278	-2.078303
18	1	-3.915177	3.659204	-0.977882
19	7	2.707899	3.580547	-1.344823

20	1	2.294806	4.055665	-2.150783
21	1	3.599825	3.938254	-0.999710
22	7	3.626753	-2.693750	-1.279114
23	1	4.114994	-2.276075	-2.074516
24	1	3.970168	-3.593613	-0.940888
25	6	-2.669725	0.213385	1.745125
26	1	-3.257725	-0.127311	2.618303
27	1	-3.396603	0.586486	1.009509
28	6	-1.743245	1.338066	2.204973
29	1	-2.354874	2.115656	2.702797
30	1	-1.051291	0.959897	2.972772
31	6	0.232263	2.701648	1.724627
32	1	-0.108470	3.309855	2.584156
33	1	0.605311	3.413682	0.972339
34	6	1.361079	1.788526	2.194087
35	1	2.148835	2.411803	2.660299
36	1	1.002443	1.114918	2.986740
37	6	2.693270	-0.208036	1.727595
38	1	3.291760	0.136245	2.592321
39	1	3.413306	-0.585988	0.986929
40	6	1.769315	-1.328459	2.199848
41	1	2.381789	-2.107022	2.695087
42	1	1.083231	-0.946721	2.971029
43	6	-0.205949	-2.694451	1.731638
44	1	0.142742	-3.300663	2.589371
45	1	-0.582090	-3.407605	0.982300
46	6	-1.333531	-1.783452	2.208302
47	1	-2.116266	-2.407380	2.681757
48	1	-0.970212	-1.106708	2.996295
49	6	-2.856380	-1.733683	0.282938
50	1	-3.523888	-1.034479	-0.248270
51	1	-3.495625	-2.399666	0.893806
52	6	-2.124376	-2.507046	-0.810576
53	6	-1.722860	2.881284	0.290247
54	1	-1.030336	3.539976	-0.262135
55	1	-2.367708	3.529748	0.914207
56	6	-2.525138	2.135842	-0.771334
57	6	2.867698	1.731052	0.257354
58	1	3.536665	1.030986	-0.271034
59	1	3.506931	2.405443	0.859179
60	6	2.126953	2.490303	-0.840001
61	6	1.740657	-2.861866	0.280722
62	1	1.046471	-3.522164	-0.267327
63	1	2.394694	-3.508075	0.897121
64	6	2.527297	-2.113546	-0.790604

E(RmPW-B95) = -1479.1978198 Hartree
Corrección de punto cero = 0.536216
Suma de las entalpías electrónicas y térmicas = -1478.628272
Suma de las energías libres y térmicas = -1478.720629

(17) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.063945	-0.040194	-0.640038
2	8	0.301638	-0.398475	-3.149484
3	1	0.592256	-1.334496	-3.010202
4	1	1.148527	0.109508	-3.182265

5	8	4.441819	0.545048	-1.304018
6	8	2.175114	0.556396	-1.414521
7	8	7.212839	-1.448743	1.559865
8	1	8.097532	-1.755057	1.870714
9	8	7.580888	-3.304841	0.308977
10	8	-0.944310	4.260090	-1.131604
11	8	-0.760230	2.011736	-1.378218
12	8	3.974873	4.076338	-0.060196
13	8	3.924610	5.502605	-1.823232
14	1	4.823659	5.103052	-1.901812
15	8	-4.473511	-0.904013	-0.615647
16	8	-2.311668	-0.769145	-1.258262
17	8	-7.895425	2.397034	-0.016513
18	8	-6.539795	3.185039	1.626654
19	1	-7.429134	3.492406	1.922700
20	8	0.674802	-4.514999	-0.797568
21	8	0.644829	-2.286755	-1.265078
22	8	-3.950245	-3.623487	-0.591509
23	8	-4.028607	-5.603436	-1.678287
24	1	-4.817730	-5.142881	-2.050360
25	7	2.023834	-0.804833	1.008744
26	7	0.823320	1.987813	0.927645
27	7	-1.987149	0.850636	1.066316
28	7	-0.816230	-1.943716	1.126316
29	6	2.251473	0.244764	2.037078
30	1	3.232791	0.107721	2.531728
31	1	1.492534	0.095900	2.823972
32	6	2.163079	1.676452	1.505467
33	1	2.920449	1.860840	0.731388
34	1	2.404927	2.366678	2.339209
35	6	-0.138192	2.260866	2.019940
36	1	0.043402	3.257722	2.470327
37	1	0.057203	1.527893	2.820405
38	6	-1.608825	2.185445	1.609783
39	1	-2.218549	2.435871	2.502422
40	1	-1.831453	2.948990	0.850966
41	6	-2.190753	-0.106757	2.180642
42	1	-3.158170	0.066605	2.694950
43	1	-1.409553	0.112019	2.926755
44	6	-2.098477	-1.583392	1.789669
45	1	-2.246244	-2.175788	2.716596
46	1	-2.922440	-1.879676	1.123758
47	6	0.227219	-2.172370	2.162472
48	1	0.070355	-1.415350	2.949829
49	1	0.081389	-3.157326	2.651678
50	6	1.673441	-2.096124	1.663747
51	1	2.329988	-2.289357	2.537402
52	1	1.865397	-2.903372	0.943497
53	6	3.215765	-1.002781	0.100062
54	1	2.939051	-1.889075	-0.501209
55	6	3.331042	0.142969	-0.947870
56	6	4.546070	-1.259906	0.829303
57	1	5.007595	-0.302348	1.116194
58	1	4.365524	-1.834802	1.756044
59	6	5.538877	-2.027116	-0.055559
60	1	5.115576	-2.975305	-0.423820
61	1	5.752710	-1.402652	-0.940440
62	6	6.862642	-2.359691	0.596342
63	6	0.917841	3.127497	-0.056246
64	1	1.733006	2.818781	-0.734809

65	6	-0.373211	3.178895	-0.931993
66	6	1.248425	4.499456	0.556449
67	1	1.908613	4.380477	1.432628
68	1	0.317390	4.997761	0.867507
69	6	1.959753	5.388201	-0.467705
70	1	2.027170	6.431334	-0.110766
71	1	1.387686	5.427072	-1.408451
72	6	3.370709	4.901254	-0.734673
73	6	-3.179493	0.991623	0.160962
74	1	-2.852845	1.751659	-0.577675
75	6	-3.282123	-0.299949	-0.647350
76	6	-4.489284	1.431989	0.837627
77	1	-4.953968	0.586587	1.370532
78	1	-4.260847	2.206532	1.586872
79	6	-5.491347	2.014241	-0.175185
80	1	-5.023139	2.865341	-0.704084
81	1	-5.777725	1.275117	-0.935812
82	6	-6.776224	2.522812	0.450581
83	6	-1.031773	-3.122132	0.215480
84	1	-1.801697	-2.767616	-0.484607
85	6	0.215259	-3.370854	-0.678741
86	6	-1.555735	-4.407902	0.874868
87	1	-2.285464	-4.174384	1.668761
88	1	-0.720396	-4.970296	1.320403
89	6	-2.215392	-5.312283	-0.174668
90	1	-1.481794	-5.517235	-0.975947
91	1	-2.478684	-6.298269	0.244625
92	6	-3.462773	-4.737714	-0.806262
93	1	-4.368783	-1.825707	-0.986555

E(RmPW-B95) = -2625.6789024 Hartree
Corrección de punto cero = 0.731857
Suma de las entalpías electrónicas y térmicas = -2624.894752
Suma de las energías libres y térmicas = -2625.033883

(18) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	0.831337	-0.022833	-0.528020
2	8	0.744573	-0.265421	-3.024100
3	7	-0.723664	1.423337	1.071064
4	6	-1.195793	0.649893	2.259563
5	1	-2.118255	1.104981	2.671594
6	1	-0.431546	0.739911	3.049092
7	6	-1.484997	-0.824453	1.977513
8	1	-2.326312	-0.903585	1.279318
9	1	-1.797105	-1.308707	2.923637
10	7	-0.321050	-1.558501	1.377689
11	6	0.639795	-1.913433	2.460309
12	1	0.237538	-2.743254	3.076209
13	1	0.707172	-1.041020	3.129354
14	6	2.034795	-2.297642	1.972769
15	1	1.982423	-3.182529	1.323063
16	1	2.646486	-2.587966	2.849570
17	7	2.693451	-1.196071	1.204579
18	6	3.236703	-0.187801	2.158784
19	1	4.167700	-0.563895	2.629882
20	1	2.506144	-0.080212	2.974482

21	6	3.526344	1.178659	1.542803
22	1	4.308339	1.095190	0.773945
23	1	3.943545	1.830838	2.335859
24	7	2.325877	1.808749	0.915357
25	6	1.440564	2.365097	1.982368
26	1	1.877172	3.297123	2.395415
27	1	1.430132	1.638036	2.809004
28	6	0.008260	2.641821	1.534166
29	1	-0.532718	3.118750	2.375802
30	1	-0.008437	3.372935	0.712107
31	6	-1.893418	1.928895	0.238426
32	1	-1.433140	2.395405	-0.649324
33	1	-2.400954	2.725904	0.815472
34	6	-2.918879	0.915912	-0.187791
35	8	-1.257710	-0.365498	-1.353465
36	6	-2.543028	-0.171146	-1.034452
37	6	-3.541841	-1.066890	-1.486119
38	1	-3.248417	-1.879277	-2.157052
39	6	-4.875490	-0.903813	-1.109962
40	1	-5.660726	-1.579692	-1.452718
41	7	-6.620492	0.330449	0.155080
42	6	-5.215369	0.158954	-0.267978
43	6	-4.256361	1.065773	0.190509
44	1	-4.583652	1.886358	0.833874
45	8	0.981806	-2.483886	-0.921915
46	7	-0.027507	-4.519835	-0.822658
47	1	0.503299	-4.857203	-1.626459
48	1	-0.728285	-5.143276	-0.423819
49	6	-0.825109	-2.764628	0.678499
50	1	-1.763253	-2.490356	0.163236
51	1	-1.065733	-3.579789	1.390765
52	6	0.122737	-3.252002	-0.410942
53	8	3.199533	-0.099460	-1.330479
54	7	5.314034	-0.936505	-1.366361
55	1	5.526564	-0.441801	-2.234050
56	1	6.031424	-1.550847	-0.983798
57	6	3.767239	-1.751663	0.351315
58	1	3.402918	-2.696596	-0.085860
59	1	4.681525	-1.983408	0.934301
60	6	4.081521	-0.851123	-0.841699
61	8	0.910165	2.262017	-1.426658
62	7	1.755362	4.354832	-1.688704
63	1	2.414583	5.085436	-1.425009
64	1	1.138081	4.532522	-2.482880
65	6	2.770968	2.871454	-0.016246
66	1	3.660956	2.504638	-0.555465
67	1	3.066846	3.794784	0.521219
68	6	1.728170	3.154480	-1.093462
69	8	-7.443358	-0.494294	-0.270290
70	8	-6.869458	1.284024	0.911913
71	1	-0.230343	-0.437240	-3.059407
72	1	1.184421	-0.956742	-3.558697

E(RmPW-B95) = -1820.4030921 Hartree
Corrección de punto cero = 0.582541
Suma de las entalpías electrónicas y térmicas = -1819.782634
Suma de las energías libres y térmicas = -1819.885240

(19) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	1.214108	-0.052441	-0.462297
2	8	0.886996	-2.309966	-0.890176
3	8	0.790846	-4.480099	-0.199595
4	8	3.005193	-0.105273	-1.946452
5	8	5.091873	-0.814846	-2.517761
6	8	0.725926	2.121424	-1.276313
7	8	1.156785	4.354885	-1.286518
8	8	-8.447045	0.026405	-0.303681
9	8	0.430224	-0.019885	-2.879631
10	7	0.113913	1.470683	1.594297
11	7	0.583644	-1.488990	1.777076
12	7	3.380831	-1.179868	0.616564
13	7	2.919947	1.779113	0.459615
14	7	-1.351839	-0.034425	-0.353551
15	7	-5.585269	-0.037312	-0.228903
16	6	-0.025312	0.701232	2.854743
17	6	-0.371963	-0.774842	2.656846
18	6	1.847821	-1.757781	2.505153
19	6	2.991940	-2.222103	1.602763
20	6	4.271873	-0.181889	1.262387
21	6	4.277851	1.185158	0.576226
22	6	2.478966	2.309357	1.769652
23	6	0.990922	2.653269	1.831228
24	6	-1.199501	1.934169	1.075369
25	6	-0.008331	-2.763385	1.286974
26	6	0.621378	-3.268033	-0.042446
27	6	4.044118	-1.784106	-0.574582
28	6	4.098980	-0.824933	-1.791546
29	6	2.906409	2.842554	-0.584892
30	6	1.481434	3.180944	-1.091350
31	6	-2.031583	0.865615	0.396295
32	6	-3.422596	0.897828	0.462673
33	6	-4.201481	-0.019706	-0.293360
34	6	-3.469232	-0.934950	-1.095422
35	6	-2.080055	-0.907281	-1.084948
36	6	-6.337786	1.189098	0.074787
37	6	-7.728789	0.849229	0.608650
38	6	-7.741514	-1.198048	-0.471623
39	6	-6.345695	-0.977936	-1.059901
40	1	1.350018	-0.200633	-3.197069
41	1	0.382912	0.969555	-2.840128
42	1	-0.796809	1.163089	3.508003
43	1	0.926723	0.786676	3.402319
44	1	-0.434203	-1.256737	3.656841
45	1	-1.368044	-0.861108	2.201665
46	1	1.678705	-2.521818	3.295155
47	1	2.145219	-0.827302	3.018088
48	1	3.854439	-2.503693	2.242136
49	1	2.698894	-3.129599	1.056599
50	1	5.313278	-0.565011	1.292339
51	1	3.953703	-0.071965	2.312083
52	1	4.956910	1.858872	1.141243
53	1	4.691359	1.092561	-0.436778
54	1	3.058901	3.220529	2.034609
55	1	2.715085	1.551710	2.537113

56	1	0.776734	3.104941	2.822676
57	1	0.756255	3.422980	1.083827
58	1	-0.974726	2.685700	0.298395
59	1	-1.788694	2.427007	1.877527
60	1	-1.075082	-2.574583	1.078686
61	1	0.055066	-3.556244	2.057001
62	1	3.433617	-2.648978	-0.884552
63	1	5.064939	-2.132154	-0.327370
64	1	3.462155	2.445945	-1.451320
65	1	3.407189	3.762072	-0.225827
66	1	-3.888583	1.642601	1.109027
67	1	-3.964885	-1.648960	-1.751574
68	1	-1.495408	-1.593329	-1.705542
69	1	-6.435981	1.805922	-0.841302
70	1	-5.805904	1.783698	0.828475
71	1	-7.635953	0.341218	1.592232
72	1	-8.317179	1.770269	0.736951
73	1	-8.340540	-1.819351	-1.154035
74	1	-7.650262	-1.722312	0.503408
75	1	-5.825328	-1.946416	-1.079479
76	1	-6.429489	-0.605268	-2.101134

E(RmPW-B95) = -1902.7251016 Hartree
Corrección de punto cero = 0.616075
Suma de las entalpías electrónicas y térmicas = -1902.070862
Suma de las energías libres y térmicas = -1902.175859

(20) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	-0.028942	-0.039162	0.038925
2	8	-0.627237	-2.018753	-1.573555
3	8	-1.210488	1.639273	-1.450261
4	8	2.091184	0.259864	1.410380
5	8	-2.435475	-2.900410	2.435543
6	8	-0.775889	-1.716210	1.429464
7	8	-2.252632	3.308558	1.205222
8	8	-1.087560	1.385508	1.576863
9	8	3.825266	0.358416	-1.784722
10	8	1.573197	0.049183	-1.664183
11	7	1.855648	-2.045669	0.077147
12	7	-2.632701	-0.493742	-0.244330
13	7	0.968073	2.519296	0.096786
14	6	1.150692	-3.251904	-0.397211
15	6	0.450716	-2.969647	-1.725295
16	6	-1.903605	-2.629974	-1.308583
17	6	-2.924783	-1.504618	-1.284489
18	6	-2.033272	-1.981516	1.721540
19	6	-3.042568	-0.986446	1.100892
20	6	-3.299837	0.796194	-0.550269
21	6	-2.634045	1.552543	-1.693932
22	6	-1.200557	2.657280	1.299261
23	6	0.166064	3.337056	1.039614
24	6	-0.652040	2.942906	-1.741027
25	6	0.805623	2.977511	-1.302166
26	6	2.399052	2.450391	0.456450
27	6	2.633940	1.569943	1.678174
28	6	2.820821	-0.293666	-1.471084

29	6	3.003073	-1.673968	-0.788946
30	6	2.822594	-0.827200	2.005759
31	6	2.225971	-2.144977	1.504160
32	1	1.848717	-4.108063	-0.527442
33	1	0.403386	-3.522993	0.365967
34	1	0.053438	-3.903717	-2.161044
35	1	1.138359	-2.508334	-2.449364
36	1	-2.149704	-3.329013	-2.130252
37	1	-1.879703	-3.195206	-0.360906
38	1	-3.940403	-1.930505	-1.145643
39	1	-2.898400	-1.008818	-2.268170
40	1	-3.068439	-0.111520	1.769539
41	1	-4.049399	-1.444255	1.066948
42	1	-4.374154	0.652113	-0.793564
43	1	-3.224194	1.427486	0.348153
44	1	-3.061694	2.569453	-1.720412
45	1	-2.785839	1.086449	-2.684635
46	1	0.697874	3.401857	2.002555
47	1	0.028216	4.367440	0.662640
48	1	-0.711905	3.141684	-2.826475
49	1	-1.258339	3.693732	-1.202895
50	1	1.164617	4.022206	-1.431901
51	1	1.410124	2.307135	-1.932154
52	1	2.944511	2.016460	-0.398252
53	1	2.819724	3.458948	0.659377
54	1	2.162816	1.967883	2.595270
55	1	3.721213	1.484248	1.852711
56	1	3.943539	-1.669812	-0.215567
57	1	3.140272	-2.431383	-1.582425
58	1	3.885047	-0.718987	1.717755
59	1	2.755903	-0.781509	3.108156
60	1	1.301883	-2.377891	2.053655
61	1	2.967697	-2.950820	1.694837

E(RmPW-B95) = -1580.9414033 Hartree
Corrección de punto cero = 0.493560
Suma de las entalpías electrónicas y térmicas = -1580.417363
Suma de las energías libres y térmicas = -1580.504015

(21) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	63	-0.116299	0.282737	-0.416799
2	8	1.239422	0.723663	-2.263868
3	8	2.867649	0.067487	-3.712116
4	8	5.344165	2.151102	0.812968
5	8	5.510641	-0.049761	0.211929
6	8	-0.107971	0.806380	1.987360
7	8	-0.873616	0.245748	4.058788
8	8	-0.049134	-2.010760	-1.292377
9	8	-0.920456	-4.057736	-1.795983
10	8	-1.957922	0.219563	-2.013387
11	8	-4.177236	0.328371	-2.518340
12	8	-0.248632	2.709986	-0.404887
13	8	-0.956004	4.720181	0.420419
14	7	2.617600	-0.251746	-0.087973
15	7	0.659557	-1.828439	1.628664
16	7	-2.191857	-1.538919	0.456841

17	7	-2.523459	1.482420	0.429180
18	6	2.337097	0.097035	-2.586920
19	6	2.991753	-0.721046	-1.448883
20	6	4.884316	1.037677	0.432755
21	6	3.310026	1.044469	0.225185
22	6	3.001206	-1.267663	0.919516
23	6	1.942556	-2.347627	1.118257
24	6	-0.177168	0.058220	3.032290
25	6	0.734311	-1.190898	2.950380
26	6	-0.378576	-2.859028	1.627090
27	6	-1.794748	-2.276528	1.668942
28	6	-0.981703	-2.901488	-1.323079
29	6	-2.334127	-2.458372	-0.696013
30	6	-3.453579	-0.811031	0.724619
31	6	-3.231732	0.576057	1.338067
32	6	-3.155713	0.674929	-1.878598
33	6	-3.290496	1.773726	-0.793269
34	6	-1.018965	3.479895	0.295542
35	6	-2.124837	2.734781	1.097129
36	1	4.091103	-0.724601	-1.550822
37	1	2.609426	-1.751169	-1.565366
38	1	3.049607	1.747609	-0.583715
39	1	2.845085	1.447470	1.144026
40	1	1.763158	-0.839129	3.123119
41	1	0.480305	-1.905454	3.764821
42	1	-2.879768	-1.917121	-1.487033
43	1	-2.913311	-3.366025	-0.411880
44	1	-2.865112	2.696465	-1.223245
45	1	-4.364979	1.959234	-0.565380
46	1	-2.992951	3.413266	1.253011
47	1	-1.689367	2.467550	2.073527
48	1	3.971227	-1.723541	0.651081
49	1	3.197535	-0.734333	1.865413
50	1	1.713557	-2.813151	0.145130
51	1	2.359352	-3.138531	1.792552
52	1	-0.251572	-3.498326	0.741800
53	1	-0.273164	-3.526159	2.521828
54	1	-1.883626	-1.599275	2.535845
55	1	-2.509905	-3.120943	1.841790
56	1	-4.002751	-0.709730	-0.224233
57	1	-4.109729	-1.404204	1.405958
58	1	-4.237668	0.986650	1.614495
59	1	-2.637450	0.505358	2.266505

E(RmPW-B95) = -1857.227736 Hartree
Corrección de punto cero = 0.434442
Suma de las entalpías electrónicas y térmicas = -1856.758371
Suma de las energías libres y térmicas = -1856.857258

(22) mPWB95/LCRECP/6-31G(d) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.102127	-1.336082	0.187006
2	6	0.806354	2.118953	-0.066402
3	6	2.218115	1.448011	-0.278696
4	6	3.047303	2.339402	-1.242494
5	6	3.294495	3.754251	-0.717417
6	6	1.957865	4.406782	-0.367124

7	6	1.178361	3.491768	0.583626
8	7	-0.203459	1.319416	0.735472
9	6	0.100191	1.384136	2.197008
10	6	1.427302	0.670976	2.544701
11	8	1.516052	-0.533650	2.066596
12	8	2.283267	1.271970	3.227201
13	7	2.265786	0.014891	-0.698373
14	6	3.469211	-0.657568	-0.166738
15	6	3.354587	-2.200777	-0.215640
16	8	2.129709	-2.657660	-0.252040
17	8	4.398820	-2.868924	-0.165255
18	6	2.217059	-0.189225	-2.165311
19	6	0.853524	0.288386	-2.681800
20	8	-0.116221	-0.258958	-2.019009
21	8	0.761518	1.128511	-3.600979
22	6	-1.672269	1.702794	0.525375
23	6	-2.352942	0.953425	-0.651268
24	6	-3.772133	1.487477	-0.971750
25	6	-3.861616	3.007544	-1.103412
26	6	-3.372905	3.630061	0.203323
27	6	-1.913077	3.230229	0.440254
28	7	-2.377141	-0.528464	-0.424702
29	6	-2.755746	-1.268932	-1.651820
30	6	-2.241821	-2.738921	-1.645468
31	8	-1.230612	-2.970318	-0.859534
32	8	-2.812465	-3.544718	-2.399219
33	6	-3.224799	-0.998012	0.696834
34	6	-2.563908	-0.817188	2.079596
35	8	-1.322322	-1.187739	2.101147
36	8	-3.229552	-0.362614	3.032162
37	8	0.740457	-3.193939	1.953280
38	1	0.351759	2.277786	-1.062080
39	1	2.711281	1.466155	0.707419
40	1	2.516355	2.388804	-2.211664
41	1	4.012610	1.835029	-1.429644
42	1	3.852637	4.351039	-1.463551
43	1	3.920453	3.708616	0.194315
44	1	1.371810	4.571310	-1.292262
45	1	2.110098	5.399209	0.097751
46	1	1.802817	3.279747	1.472964
47	1	0.293176	4.018346	0.954405
48	1	-0.694547	0.828472	2.719199
49	1	0.120489	2.421873	2.577720
50	1	3.566832	-0.389223	0.896990
51	1	4.392664	-0.349301	-0.701199
52	1	2.291056	-1.277405	-2.329732
53	1	3.059319	0.298838	-2.692963
54	1	-2.170752	1.372175	1.452325
55	1	-1.716287	1.083147	-1.545251
56	1	-4.469082	1.187369	-0.168584
57	1	-4.121011	0.991338	-1.893258
58	1	-4.899573	3.314089	-1.332658
59	1	-3.228455	3.362485	-1.939258
60	1	-4.004849	3.271338	1.038253
61	1	-3.457233	4.732918	0.186272
62	1	-1.313555	3.653066	-0.386856
63	1	-1.556966	3.692897	1.376363
64	1	-2.285721	-0.763757	-2.508999
65	1	-3.853700	-1.287662	-1.804571
66	1	-3.336675	-2.085967	0.548823

67	1	-4.240300	-0.557279	0.694137
68	1	1.513614	-3.348579	1.347291
69	1	1.021213	-2.415636	2.496058

E(RmPW-B95) = -1885.1241016 Hartree
Corrección de punto cero = 0.542140
Suma de las entalpías electrónicas y térmicas = -1884.545136
Suma de las energías libres y térmicas = -1884.646417

$[Gd(dpa12c4)]^{+\cdot}$ HCO_3^- (vacío) **Δ(λλλλ)** (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.063774	0.256807	-0.029672
2	7	1.248412	-2.328222	0.610301
3	6	1.981652	-2.840681	-0.578800
4	6	1.951279	-1.927210	-1.819236
5	6	0.378210	-0.784298	-3.253126
6	6	-0.854926	0.147436	-3.173325
7	7	-1.773889	-0.230213	-2.076499
8	6	-2.313629	-1.594142	-2.256386
9	6	-2.716454	-2.270721	-0.946168
10	6	-0.929808	-3.480327	0.097838
11	6	0.217400	-3.281441	1.074188
12	6	2.137042	-2.005857	1.754899
13	6	-2.851159	0.764514	-1.854648
14	1	1.560917	-3.812792	-0.855635
15	1	3.035640	-3.022636	-0.330497
16	1	2.677582	-1.113830	-1.753253
17	1	2.180378	-2.535137	-2.706209
18	1	0.223251	-1.611902	-3.958953
19	1	1.237066	-0.190531	-3.579514
20	1	-0.514741	1.166446	-2.970930
21	1	-1.352982	0.144609	-4.158136
22	1	-1.544701	-2.207624	-2.727720
23	1	-3.182337	-1.582254	-2.938067
24	1	-3.560106	-1.765072	-0.471962
25	1	-3.030451	-3.301917	-1.159755
26	1	-0.574860	-3.812693	-0.888842
27	1	-1.591128	-4.265756	0.495255
28	1	-0.199934	-2.880314	2.000906
29	1	0.660650	-4.269060	1.295607
30	1	1.485930	-1.691913	2.578499
31	1	2.706770	-2.891552	2.084650
32	1	-2.439912	1.755473	-2.060173
33	1	-3.696344	0.593419	-2.541221
34	8	0.646041	-1.352780	-1.957671
35	8	-1.640047	-2.257889	-0.013781
36	6	3.084046	-0.876580	1.417448
37	6	4.374966	-0.752296	1.934456
38	6	5.158756	0.327213	1.516117
39	1	4.758558	-1.484269	2.639176
40	6	3.372169	1.001122	0.071473
41	6	4.663084	1.208636	0.555890
42	1	6.162696	0.454074	1.912807
43	1	5.244494	2.028915	0.150743
44	6	-3.340170	0.758316	-0.411922
45	6	-4.658583	1.032767	-0.044666
46	6	-2.738186	0.388724	1.813440

47	6	-4.998878	0.996150	1.311937
48	1	-5.403617	1.262434	-0.801021
49	6	-4.034510	0.654801	2.258508
50	1	-6.018294	1.213109	1.620215
51	1	-4.249228	0.576534	3.317978
52	7	-2.417365	0.470322	0.516064
53	7	2.599954	0.009395	0.540533
54	6	2.790209	1.777479	-1.114700
55	8	1.657391	1.307233	-1.521431
56	8	3.456268	2.693611	-1.589693
57	6	-1.622257	-0.077845	2.757971
58	8	-1.907634	-0.269609	3.935447
59	8	-0.474304	-0.260559	2.181225
60	8	0.545667	2.418290	0.998407
61	6	-0.159484	3.056217	0.154227
62	8	-0.848635	2.489552	-0.735990
63	8	-0.187269	4.403837	0.209903
64	1	0.418952	4.654292	0.928436

E(RB3LYP) = -1824.9071629 Hartree
Corrección de punto cero = 0.507084
Suma de las entalpías electrónicas y térmicas = -1824.365808
Suma de las energías libres y térmicas = -1824.463411

[Gd(dpa12c4)]$^{+\cdot}$ $H_2PO_4^-$ (vacío) Δ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico	Coordenadas (Angstroms) X	Y	Z
1	64	0.067781	0.116632	-0.028555
2	7	1.206869	-2.600958	0.457036
3	6	1.899397	-3.047297	-0.780369
4	6	1.870815	-2.043952	-1.949033
5	6	0.246458	-0.856233	-3.292132
6	6	-1.019596	0.023831	-3.158086
7	7	-1.882509	-0.406203	-2.037044
8	6	-2.402675	-1.771315	-2.244630
9	6	-2.822501	-2.469112	-0.952086
10	6	-1.001145	-3.718743	-0.044751
11	6	0.181758	-3.572506	0.896736
12	6	2.129590	-2.371880	1.593916
13	6	-2.971444	0.556754	-1.742619
14	1	1.441707	-3.982252	-1.119203
15	1	2.952379	-3.280485	-0.571246
16	1	2.622386	-1.258079	-1.844287
17	1	2.058486	-2.591520	-2.883405
18	1	0.098196	-1.684306	-3.998966
19	1	1.073541	-0.232403	-3.646659
20	1	-0.724281	1.054410	-2.948986
21	1	-1.548916	0.009293	-4.126802
22	1	-1.618512	-2.369659	-2.712089
23	1	-3.259873	-1.759534	-2.941907
24	1	-3.646173	-1.946399	-0.461550
25	1	-3.174792	-3.483320	-1.190340
26	1	-0.679203	-3.958170	-1.069233
27	1	-1.622905	-4.556975	0.308419
28	1	-0.203086	-3.224305	1.858660
29	1	0.628337	-4.571872	1.050125
30	1	1.508632	-2.081118	2.448822

31	1	2.674682	-3.293711	1.862076
32	1	-2.603937	1.557779	-1.976355
33	1	-3.857072	0.355361	-2.367408
34	8	0.580263	-1.423019	-2.012989
35	8	-1.749557	-2.516616	-0.020101
36	6	3.109684	-1.258703	1.311266
37	6	4.412317	-1.221436	1.816928
38	6	5.223933	-0.131734	1.494200
39	1	4.779033	-2.026093	2.447332
40	6	3.441606	0.726399	0.151743
41	6	4.737662	0.862026	0.643955
42	1	6.235221	-0.071748	1.887436
43	1	5.330412	1.718808	0.344581
44	6	-3.364063	0.548980	-0.271726
45	6	-4.661644	0.816153	0.170358
46	6	-2.641495	0.176889	1.916483
47	6	-4.927042	0.778400	1.542416
48	1	-5.448384	1.041036	-0.544076
49	6	-3.910999	0.436558	2.433059
50	1	-5.928601	0.991557	1.906767
51	1	-4.066431	0.351755	3.502269
52	7	-2.387843	0.268991	0.603068
53	7	2.645418	-0.290247	0.517097
54	6	2.815571	1.663398	-0.867899
55	8	1.804912	1.168969	-1.476102
56	8	3.296603	2.802443	-1.005938
57	6	-1.483133	-0.305620	2.797163
58	8	-1.699420	-0.492376	3.989047
59	8	-0.374341	-0.514667	2.152672
60	8	0.633209	2.214100	1.006258
61	8	-0.835815	2.252008	-0.992113
62	15	-0.054476	3.135925	-0.017086
63	8	0.964282	4.172557	-0.684044
64	8	-1.117048	4.148179	0.672284
65	1	-0.654913	4.818237	1.202621
66	1	1.836651	3.751518	-0.935052

E(RB3LYP) = -2204.0639637 Hartree
Corrección de punto cero = 0.517994
Suma de las entalpías electrónicas y térmicas = -2203.510220
Suma de las energías libres y térmicas = -2203.609714

[Gd(dpa12c4)]$^{+\cdot}$ HPO$_4^{2-}$ (vacío) Δ(λλλλ) (0 frecuencias imaginarias)

Número Centro	Número Atómico		Coordenadas (Angstroms) X	Y	Z
1	64	0	0.310849	0.667535	0.093879
2	7	0	1.051333	-2.699213	-0.132187
3	6	0	1.610522	-2.842314	-1.486631
4	6	0	1.726121	-1.518657	-2.266313
5	6	0	-0.365713	-0.897326	-3.283218
6	6	0	-1.663514	-0.125710	-3.054107
7	7	0	-2.394258	-0.578437	-1.869828
8	6	0	-3.070070	-1.854149	-2.057173
9	6	0	-3.259537	-2.678136	-0.773762
10	6	0	-1.189863	-3.839466	-0.572960
11	6	0	0.123305	-3.796771	0.199517
12	6	0	2.052807	-2.655411	0.950398

13	6	0	-3.228789	0.447953	-1.233601
14	1	0	0.961025	-3.514071	-2.055979
15	1	0	2.606352	-3.321076	-1.474201
16	1	0	2.530299	-0.898626	-1.874117
17	1	0	1.957099	-1.739262	-3.318293
18	1	0	-0.551124	-1.972470	-3.428543
19	1	0	0.110468	-0.515913	-4.198840
20	1	0	-1.405613	0.924928	-2.900563
21	1	0	-2.257899	-0.213070	-3.986627
22	1	0	-2.490369	-2.448316	-2.771942
23	1	0	-4.074266	-1.725665	-2.515557
24	1	0	-3.940198	-2.169339	-0.088905
25	1	0	-3.722254	-3.644802	-1.044738
26	1	0	-1.026492	-3.683099	-1.649309
27	1	0	-1.619634	-4.852995	-0.463612
28	1	0	-0.137066	-3.700612	1.257870
29	1	0	0.627797	-4.776813	0.077298
30	1	0	1.507306	-2.396536	1.865848
31	1	0	2.514637	-3.651868	1.092959
32	1	0	-2.775167	1.424789	-1.431266
33	1	0	-4.255445	0.449577	-1.645697
34	8	0	0.538427	-0.727145	-2.185310
35	8	0	-2.069969	-2.882242	-0.036609
36	6	0	3.168293	-1.648385	0.796518
37	6	0	4.485854	-2.010273	1.093522
38	6	0	5.492828	-1.047047	1.017155
39	1	0	4.710830	-3.032093	1.384991
40	6	0	3.825529	0.521921	0.308504
41	6	0	5.159921	0.239703	0.613023
42	1	0	6.521187	-1.307959	1.256281
43	1	0	5.883163	1.039544	0.506180
44	6	0	-3.303042	0.291298	0.276198
45	6	0	-4.518763	0.382832	0.961116
46	6	0	-2.168945	-0.141191	2.255106
47	6	0	-4.536879	0.207068	2.344633
48	1	0	-5.432205	0.586450	0.409243
49	6	0	-3.347051	-0.087264	3.002112
50	1	0	-5.472103	0.280826	2.895137
51	1	0	-3.288829	-0.276517	4.067405
52	7	0	-2.149651	0.068753	0.928289
53	7	0	2.850135	-0.397358	0.420162
54	6	0	3.438634	1.905783	-0.225291
55	8	0	2.195170	2.024440	-0.521912
56	8	0	4.338736	2.738680	-0.340875
57	6	0	-0.845229	-0.499918	2.934969
58	8	0	-0.884127	-0.902376	4.098105
59	8	0	0.202180	-0.374949	2.187159
60	8	0	-0.348648	2.619426	0.988597
61	8	0	-0.721594	2.102970	-1.373242
62	15	0	-0.854316	3.324285	-0.346675
63	8	0	0.336020	4.367243	-0.770677
64	8	0	-2.180550	4.009984	-0.324416
65	1	0	1.172298	3.856791	-0.763070

E(RB3LYP) = -2203.5078235 Hartree
Corrección de punto cero = 0.504484
Suma de las entalpías electrónicas y térmicas = -2202.967492
Suma de las energías libres y térmicas = -2203.069414