Axial Chirality at The Boron-Carbon Bond: Synthesis, Stereodynamic Analysis and Atropisomeric Resolution of 6-Aryl-5,6-dihydrodibenzo-[*c,e*]-[1,2]-azaborinines.

Andrea Mazzanti, Maria Boffa, Emanuela Marotta and Michele Mancinelli*

Department of Industrial Chemistry "Toso Montanari", University of Bologna, Viale del Risorgimento 4, Bologna 40136, Italy

michele.mancinelli@unibo.it

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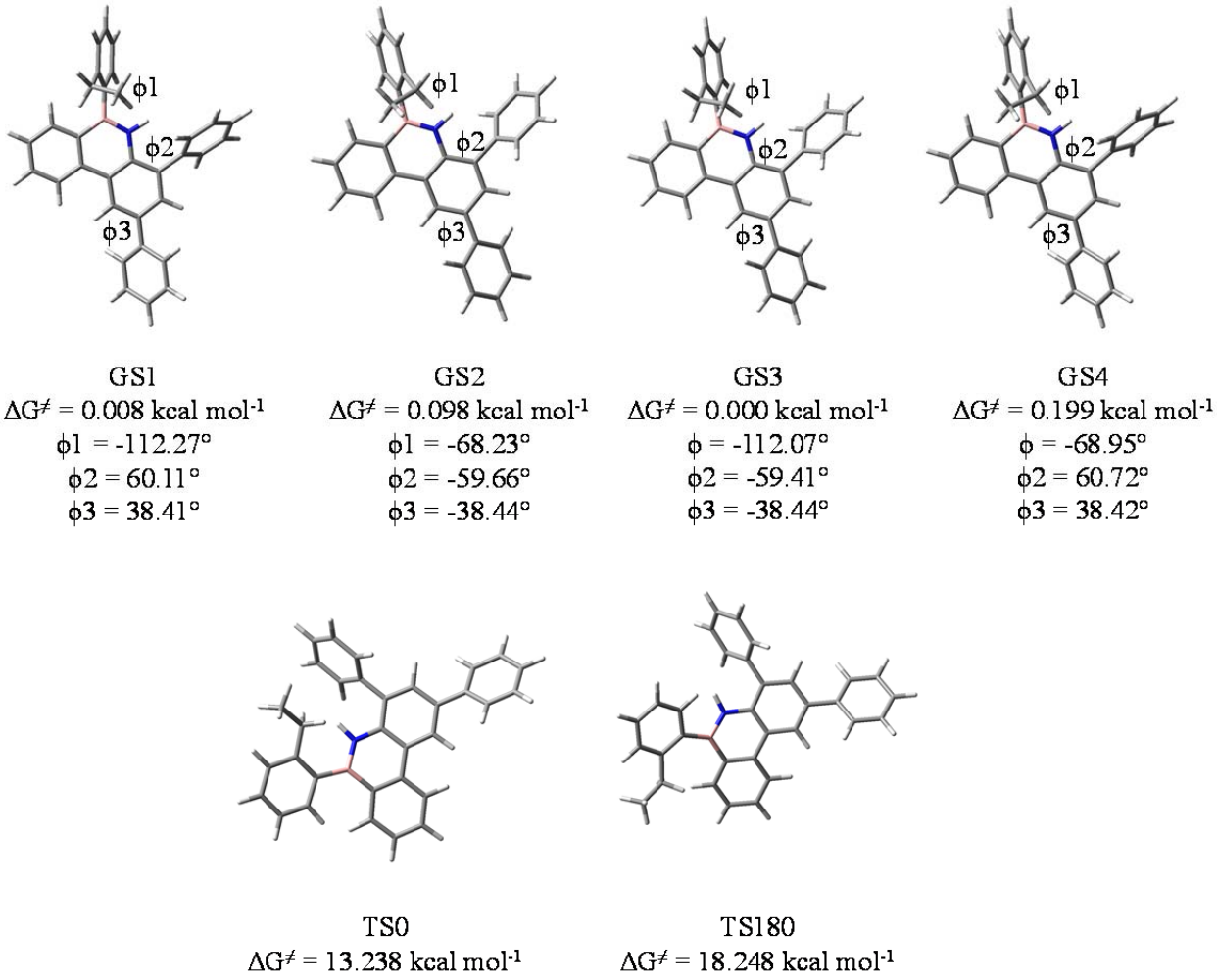
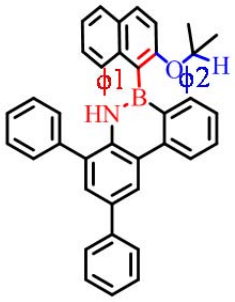
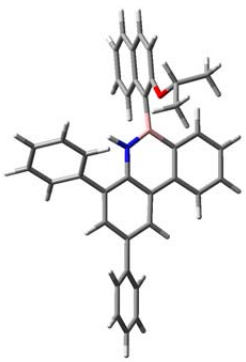
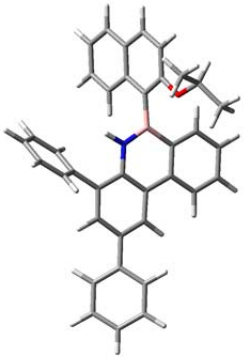


Figure S1. Ground and transition states of compound **1b**.

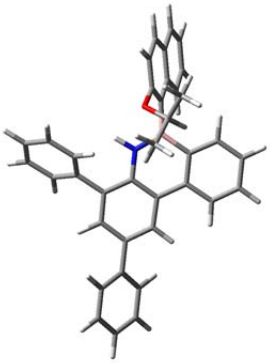




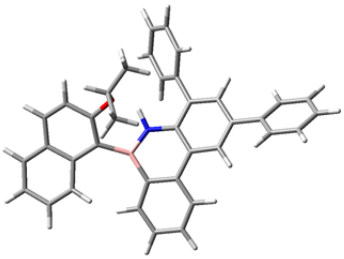
GS1
$\Delta G^{\neq}$ = 0.000 kcal mol^{-1}
ϕ1 = 79.438°
ϕ2 = 52.67°



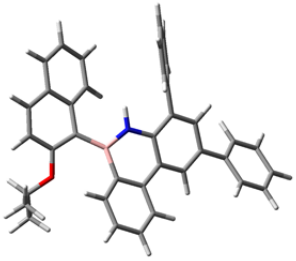
GS2
$\Delta G^{\neq}$ = 0.006 kcal mol^{-1}
ϕ1 = 105.23°
ϕ2 = -38.29°



GS3
$\Delta G^{\neq}$ = 0.961 kcal mol^{-1}
ϕ = 66.49°
ϕ2 = -45.79°



TS0
$\Delta G^{\neq}$ = 24.209 kcal mol^{-1}



TS180
$\Delta G^{\neq}$ = 21.465 kcal mol^{-1}

Figure S2. Ground and transition states of compound **1c**.

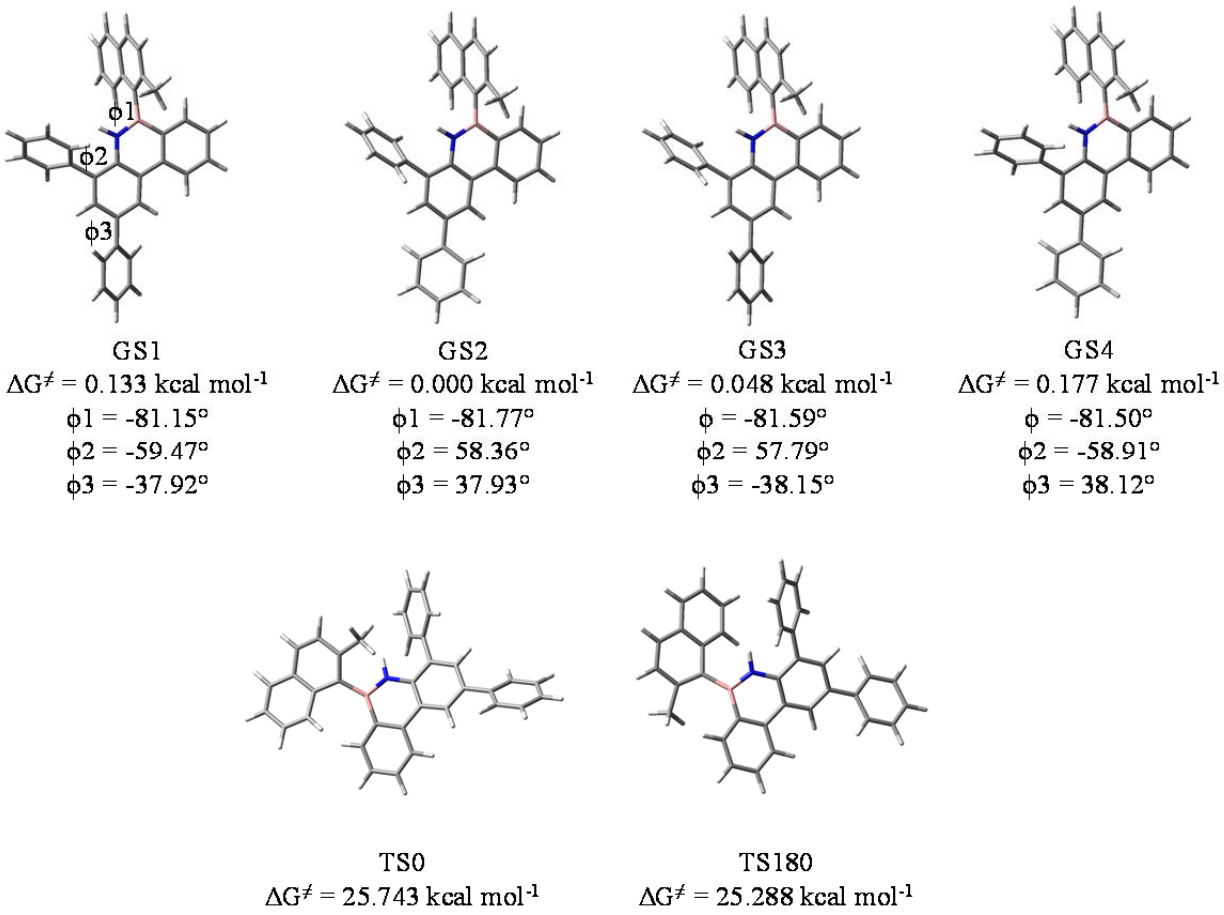


Figure S3. Ground and transition states of compound **1d**.

T(K)	1/T	ΔG1-2	ΔG2-1		ΔGaverage/T	ΔG1-2/T	ΔG2-1/T
288,15	0,00347	21,159	21,2081	21,18355	0,073515704	0,073431	0,073601
298,15	0,003354	21,5196	21,5759	21,54775	0,072271508	0,072177	0,072366
308,15	0,003245	21,8599	21,9193	21,8896	0,071035535	0,070939	0,071132
313,15	0,003193	22,0321	22,093	22,06255	0,070453616	0,070356	0,070551
318,15	0,003143	22,0938	22,1562	22,125	0,069542669	0,069445	0,069641

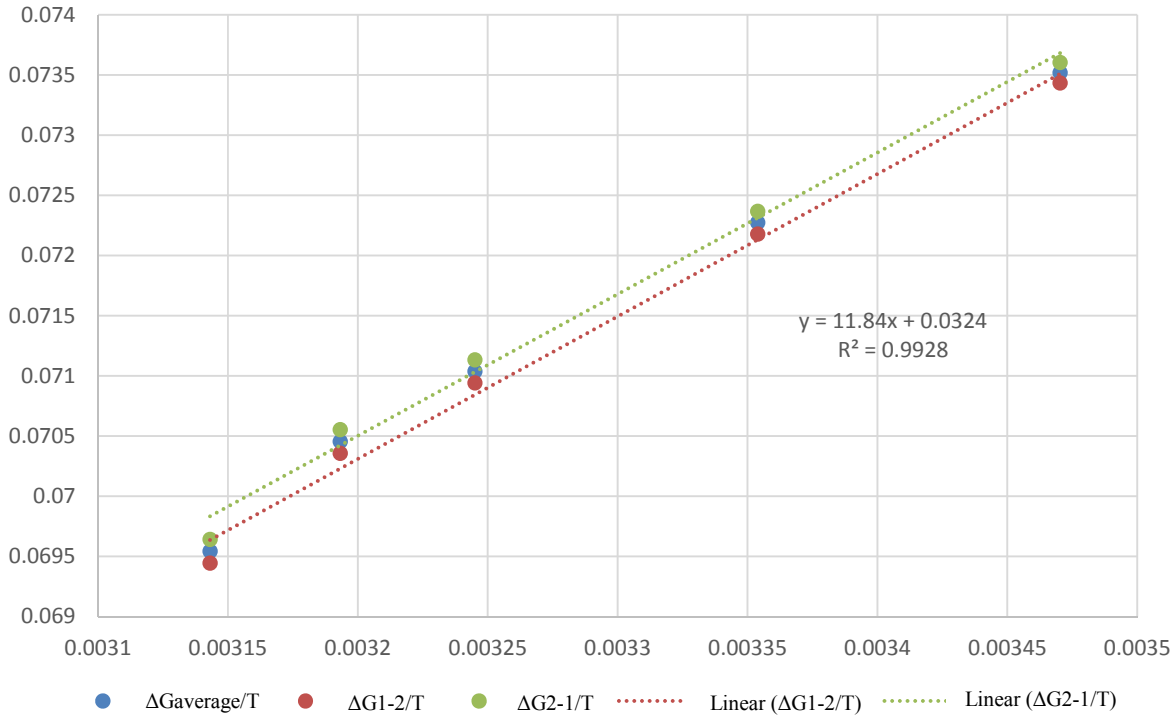


Figure S4. Dynamic HPLC data simulation of compound **1c**.

T (°C)	t (s)	$ln(x_0 - x_{eq})$	$x_{1°\ eluted}$	$x_{2°\ eluted}$
+50	0	-0.76852	96.37 %	4.63 %
	1800	-0.81193	94.4 %	5.60 %
	3720	-0.87155	91.83 %	8.17 %
	6420	-0.97206	87.83 %	12.17%
	9120	-1.09512	83.45 %	16.55 %
+45	0	-0.78679	95.53 %	4.47 %
	3720	-0.84444	92.98 %	7.02 %
	7440	-0.91604	90.01 %	9.99 %
	10440	-0.97418	87.75 %	12.25 %
	15540	-1.07441	84.15 %	15.85 %

	T = +50 °C	**T = +45 °C**
k_{Tc} (s^{-1})	$1.80 \cdot 10^{-5}$	$9.34 \cdot 10^{-6}$
$\Delta G^{\neq}$ (kcal/mol)	25.97	25.98

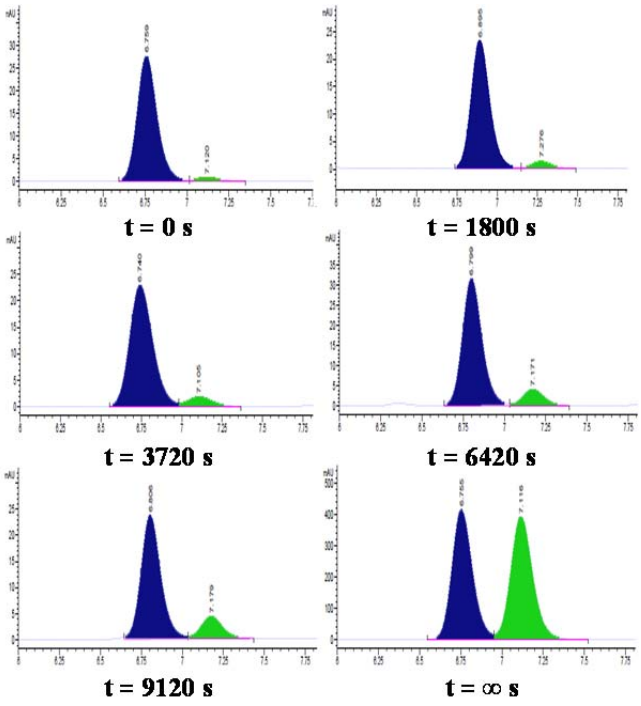


Figure S5. Kinetic racemization of compound **1d** at +45 °C and +50 °C.

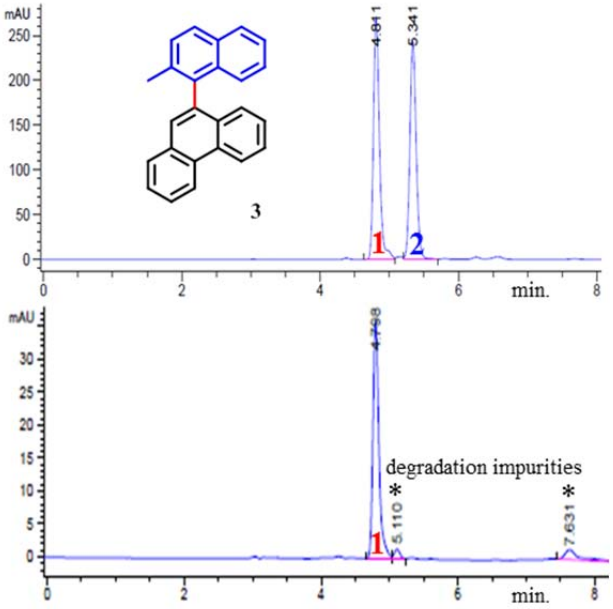


Figure S6. Kinetic racemization of compound **3** (ChiralPak AD–H, *n*-hexane/*iso*-propanol 95:5). Top: CSP-HPLC chromatogram of the racemic mixture. Bottom: chromatogram recorded after keeping the enantiopure, first eluted, atropisomer at +146.5 °C in 1,1,2,2-tretrachloroethane for 24 h.

UV and ECD of compounds 1d and 3.

The ECD spectra of compounds **1d** and **3** were acquired in the 190-400 nm region using a JASCO J-810 spectropolarimeter in HPLC-grade acetonitrile solution (Figure S7 and S8 bottom, respectively). Concentration was about $1 \cdot 10^{-4}$ M, optimized in order to have a maximum absorbance between 0.8 and 1 (UV/vis in figure S7 up and S8 middle, respectively), with a cell path of 0.2 cm. The spectrum was obtained by the average of 16 scans at 50 nm·min^{-1} scan rate.

The ECD spectrum for compounds **1d** shows a large negative band at 235 nm and a positive one at 225 nm due to the naphthyl and to the 1,2-dibenzoazaborinine chromophores.

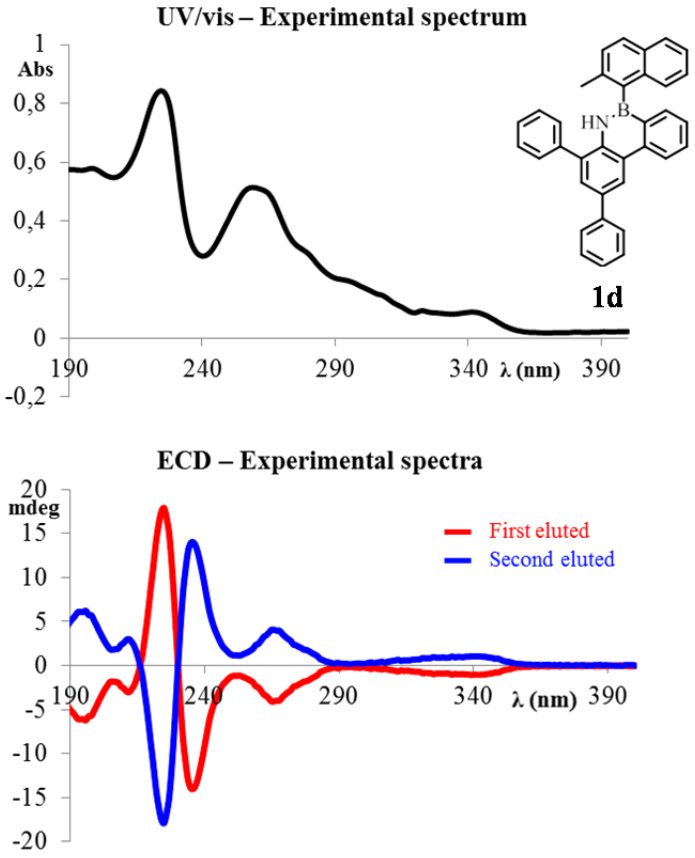


Figure S7. Up: experimental UV/Vis spectrum of compound **1d**. Bottom: experimental ECD spectra of first and second CSP-HPLC eluted **1d** (for the HPLC elution see figure 4 in the text).

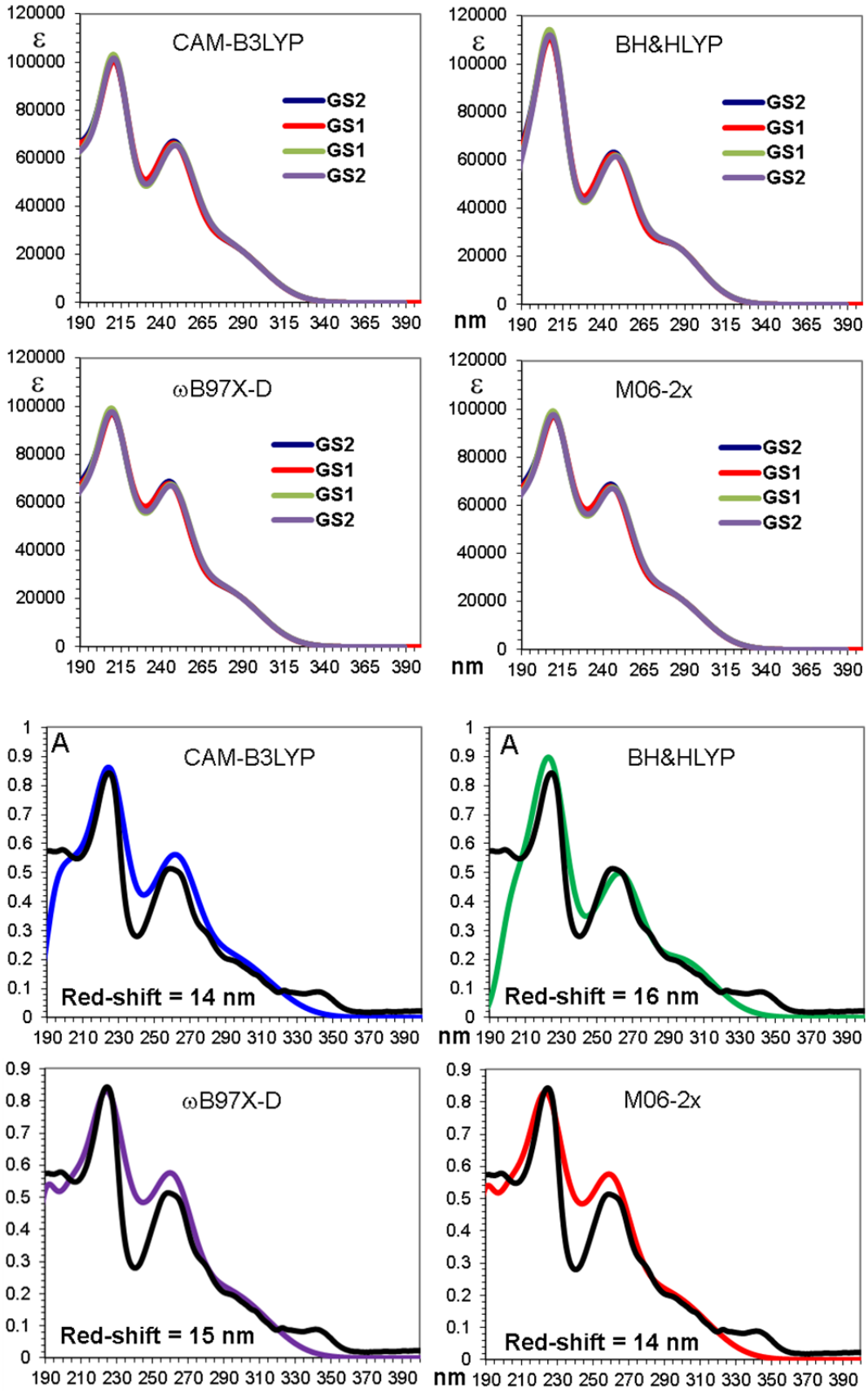


Figure S8. Top: UV simulations of the four conformations of **1d**. Bottom: Boltzmann averaged UV spectra (colored traces) compared with the experimental UV spectrum of g.

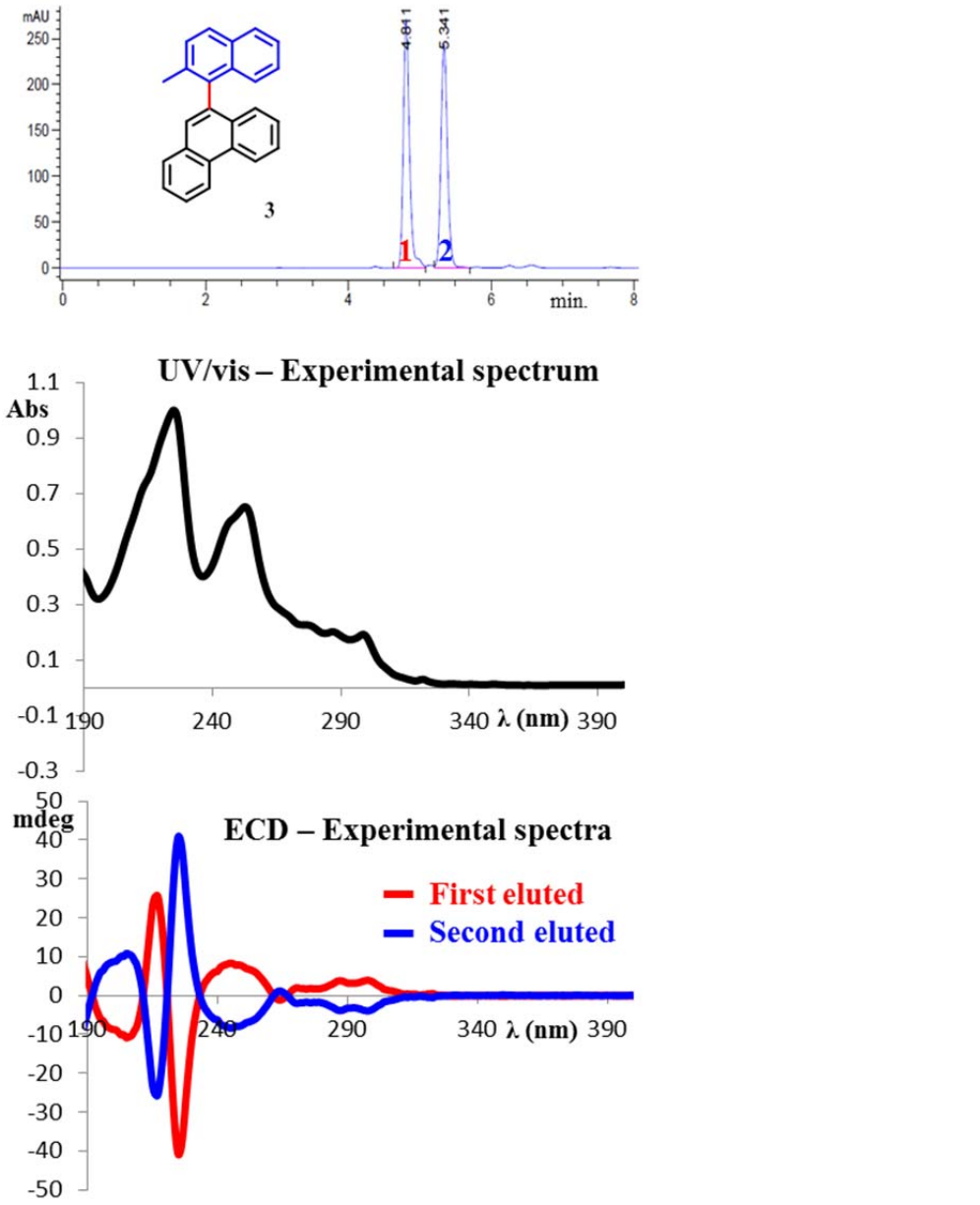


Figure S9. Top: CSP-HPLC chromatogram of compound **3** (ChiralPak AD–H, *n*-hexane/*iso*-propanol 95:5). Middle: experimental UV/Vis spectrum. Bottom: experimental ECD spectra of first and second CSP-HPLC eluted**.**

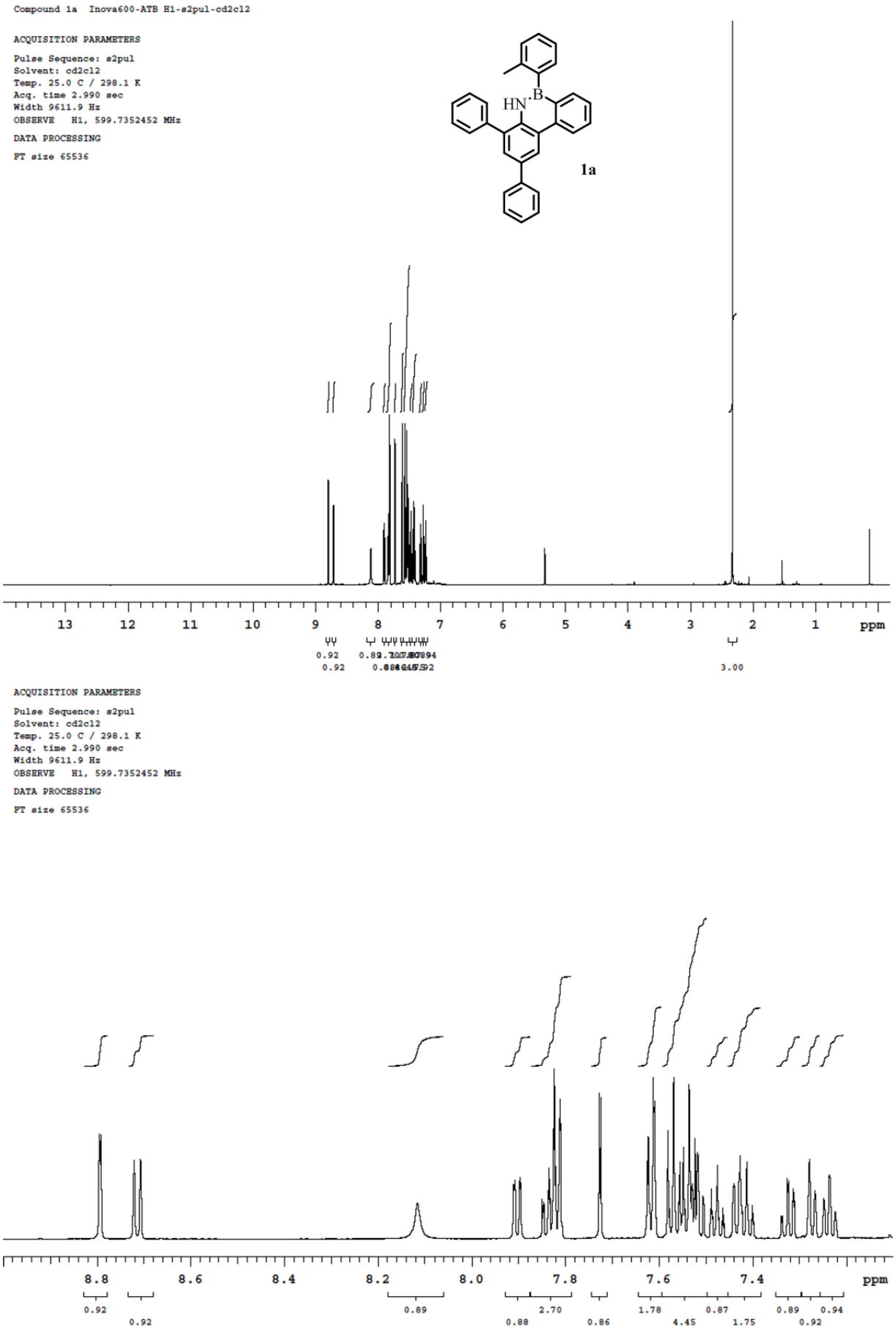


Figure S10. Up: ^{1}H NMR at 600 MHz in CD_2Cl_2 of compound **1a**. Bottom: Zoom of aromatic region.

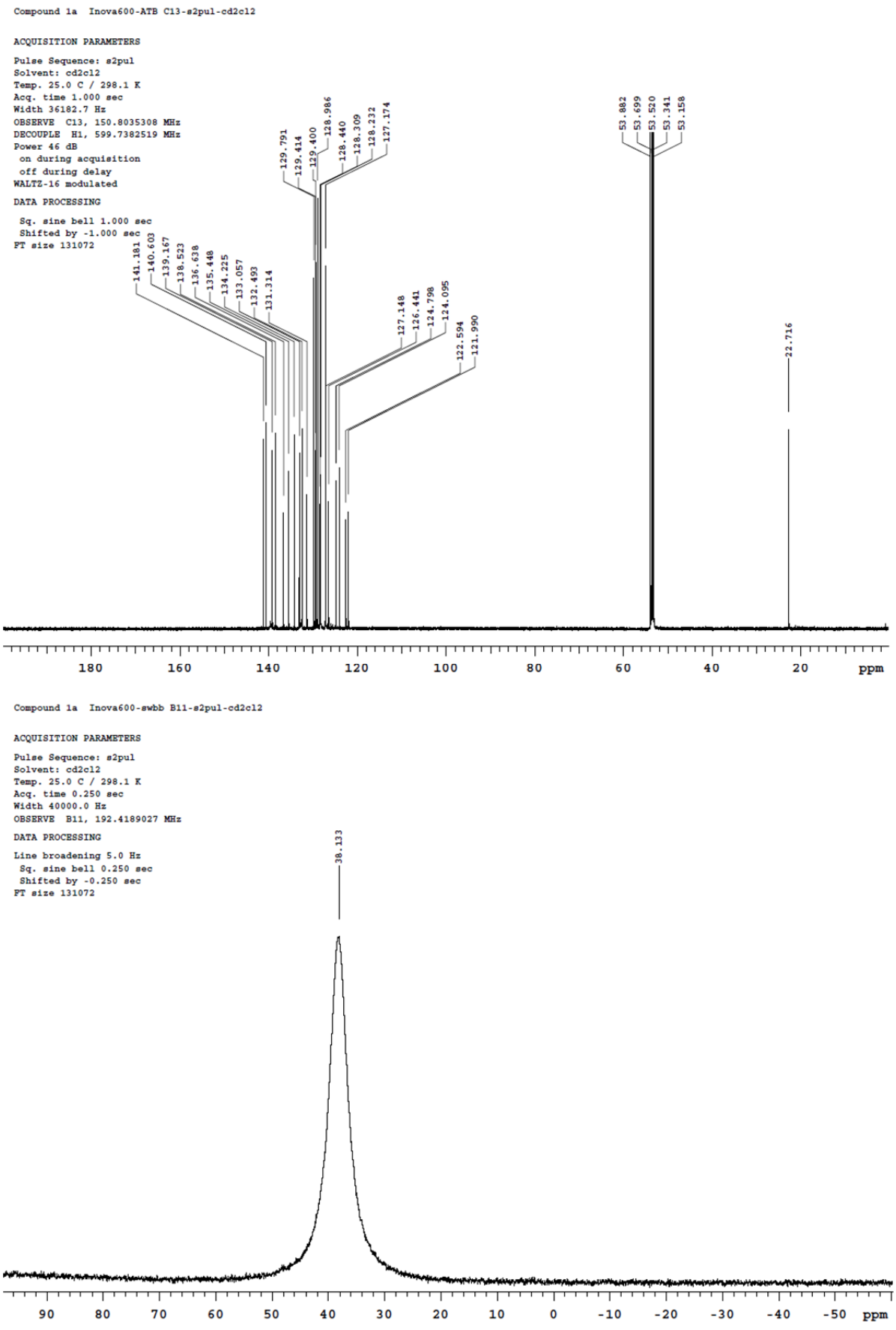


Figure S11. Compound **1a.** Up: ^{13}C NMR at 150.8 MHz, and bottom: ^{11}B NMR at 192.4 MHz in CD_2Cl_2.

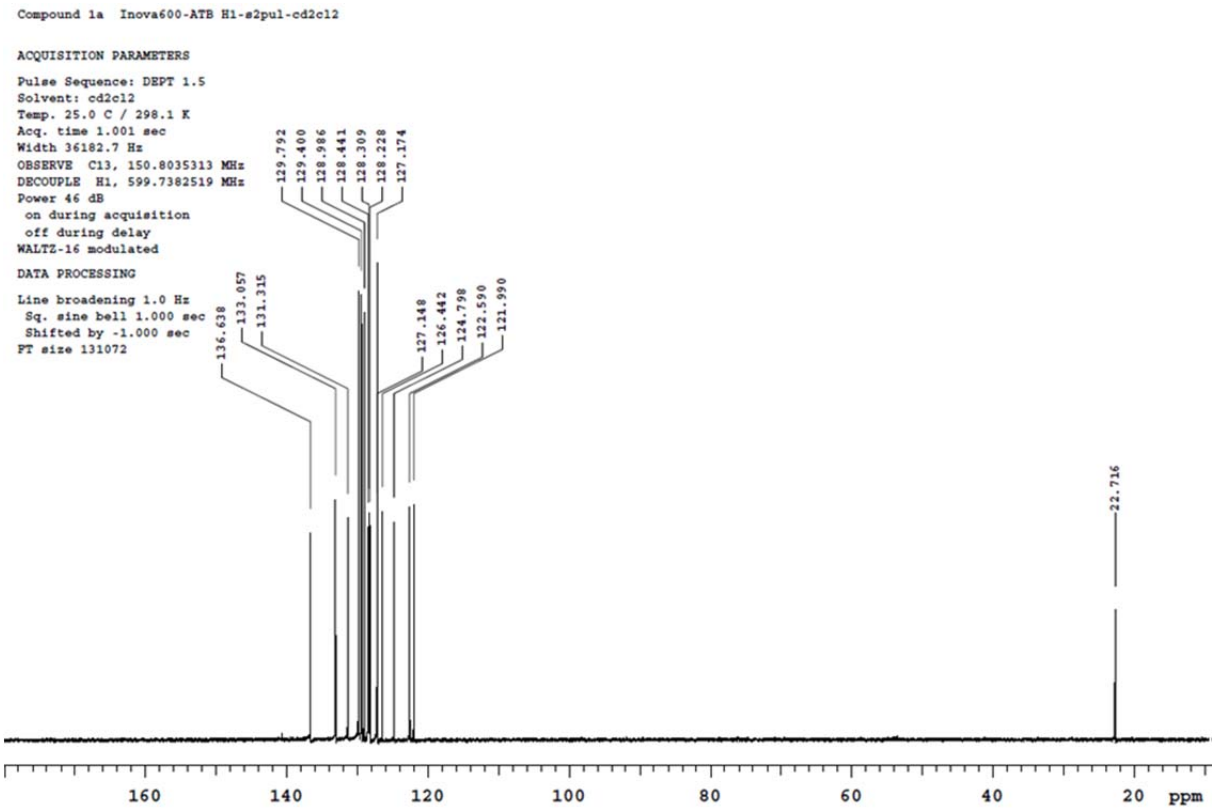


Figure S12. Compound **1a.** DEPT-135 at 150.8 MHz, in CD_2Cl_2.

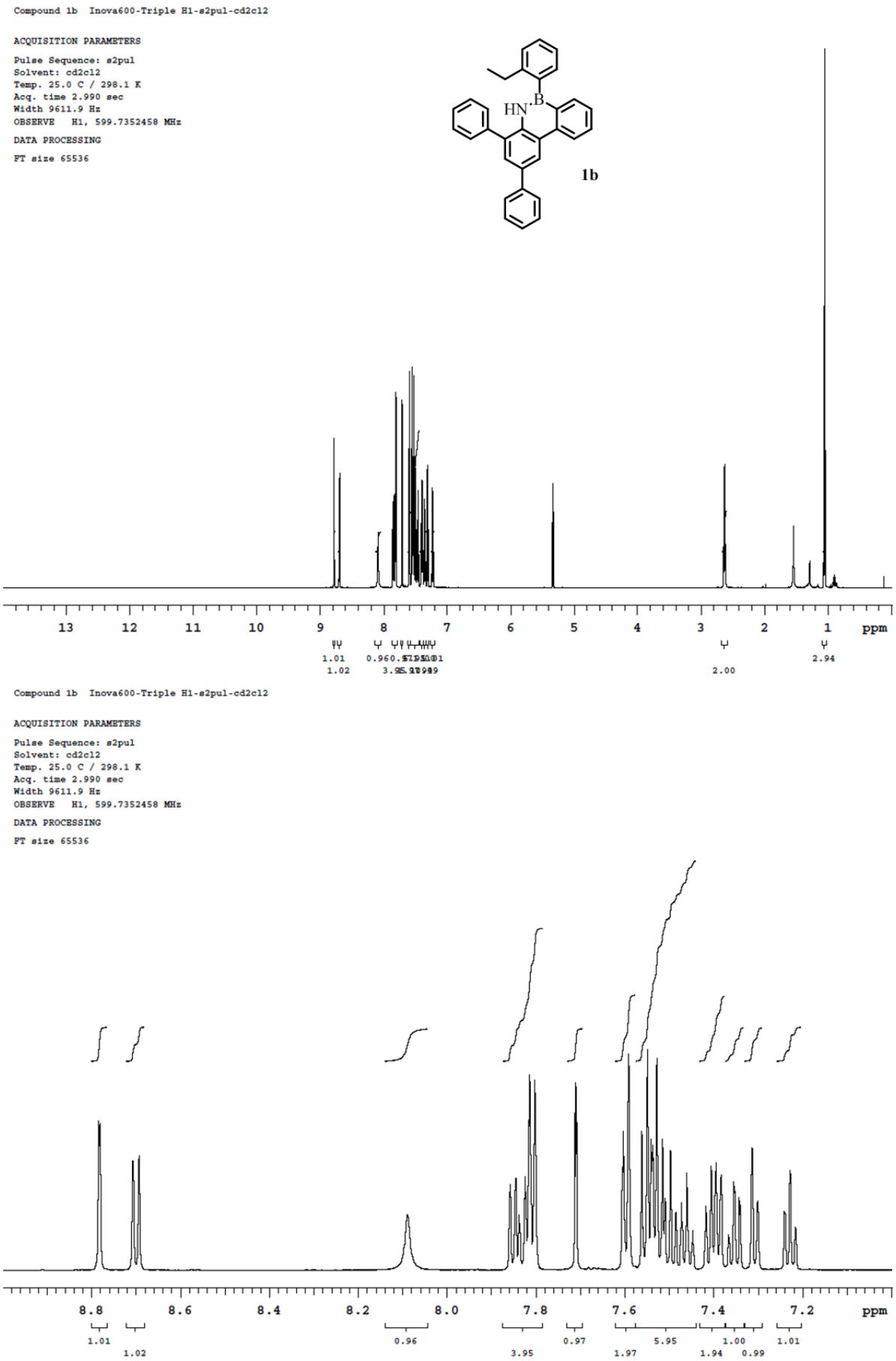


Figure S13. Up: ^{1}H NMR at 600 MHz in CD_2Cl_2 of compound **1b**. Bottom: Zoom of aromatic region.

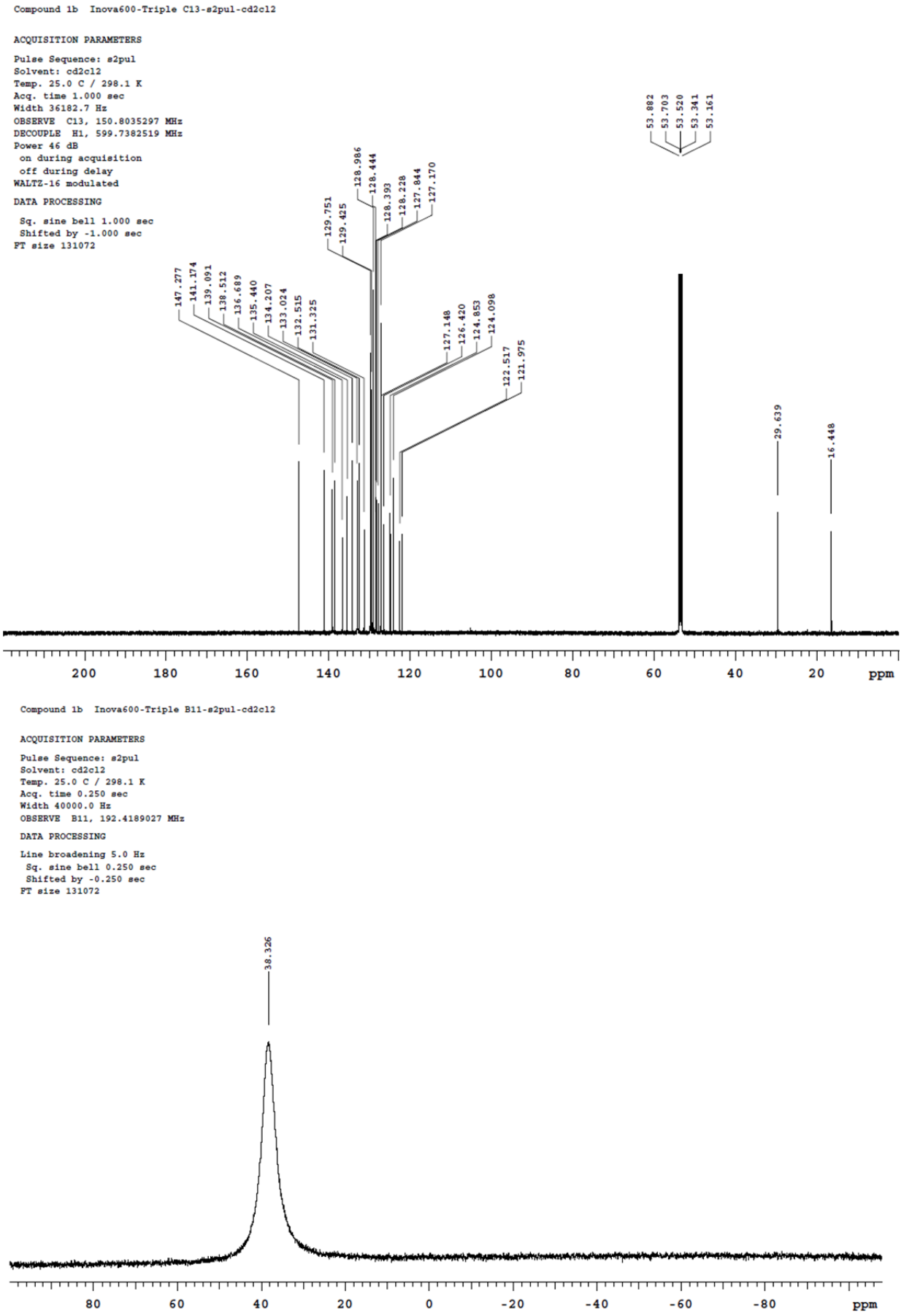


Figure S14. Compound **1b.** Up: ^{13}C NMR at 150.8 MHz, and bottom: ^{11}B NMR at 192.4 MHz in CD_2Cl_2.

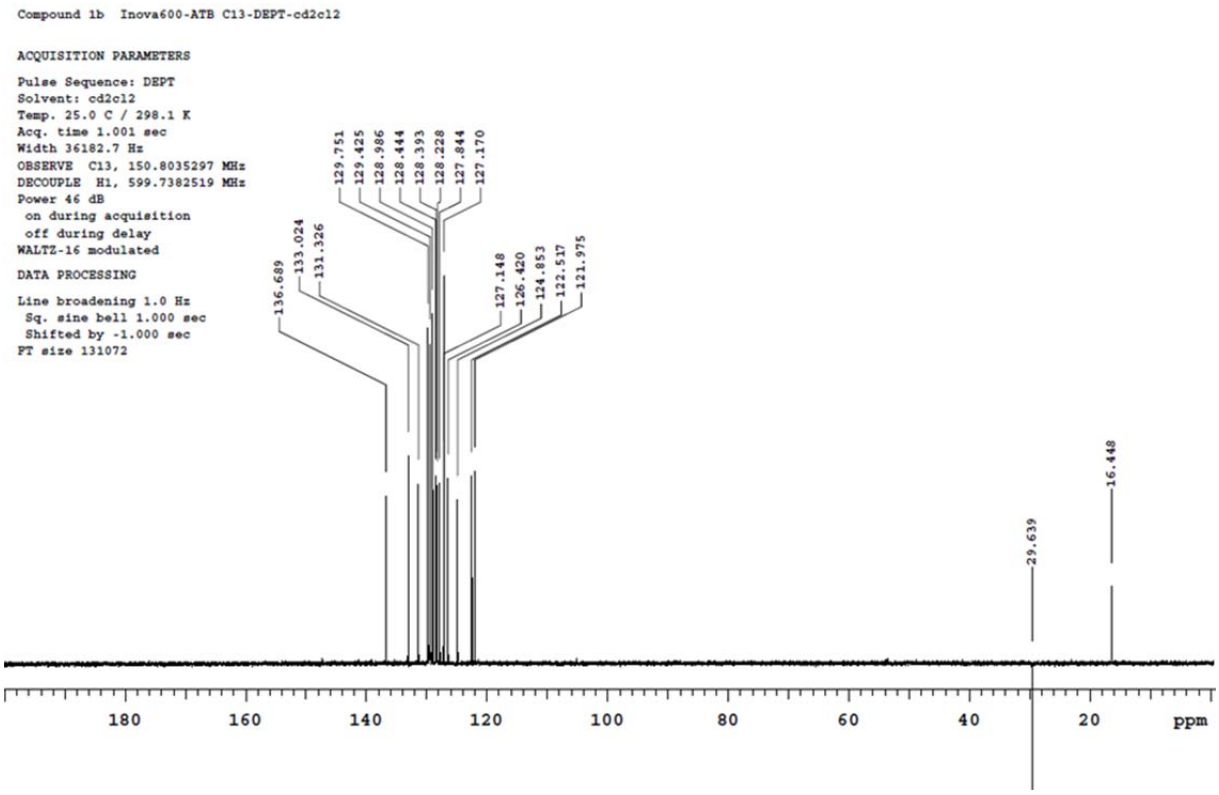
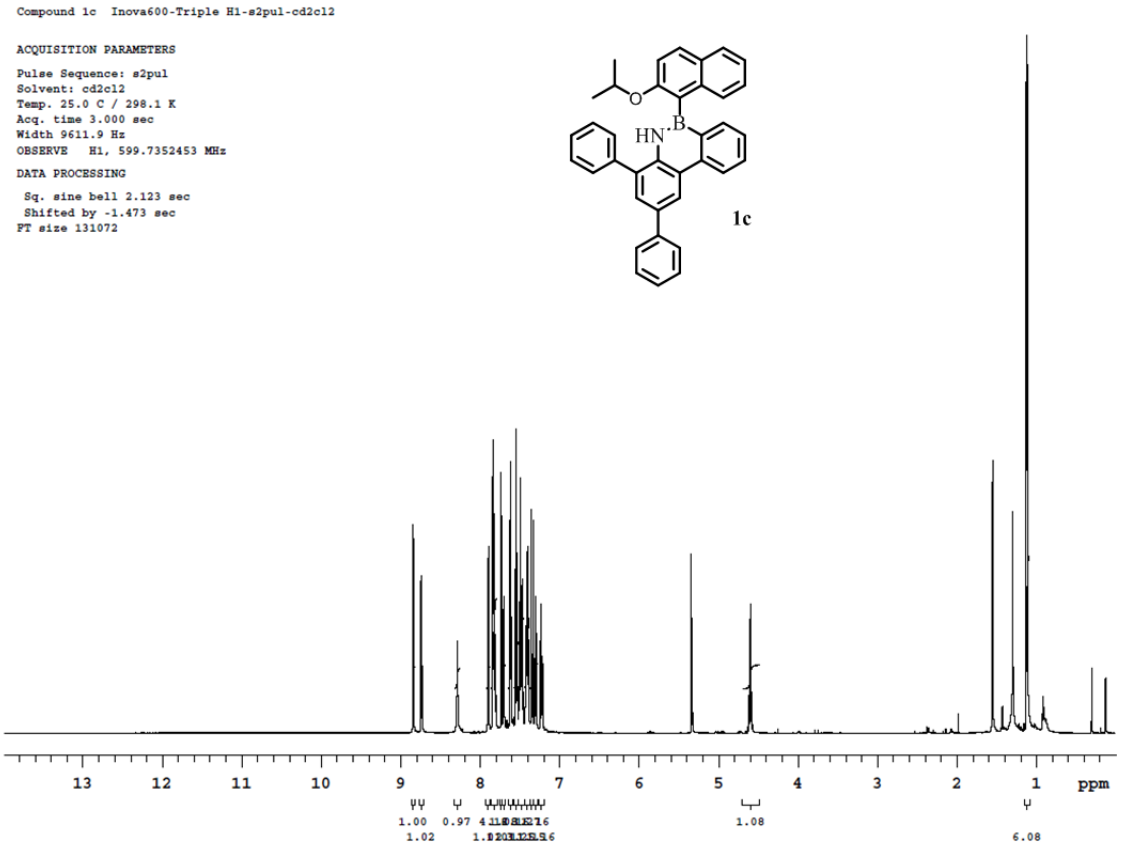


Figure S15. Compound **1b.** DEPT-135 at 150.8 MHz, in CD_2Cl_2.



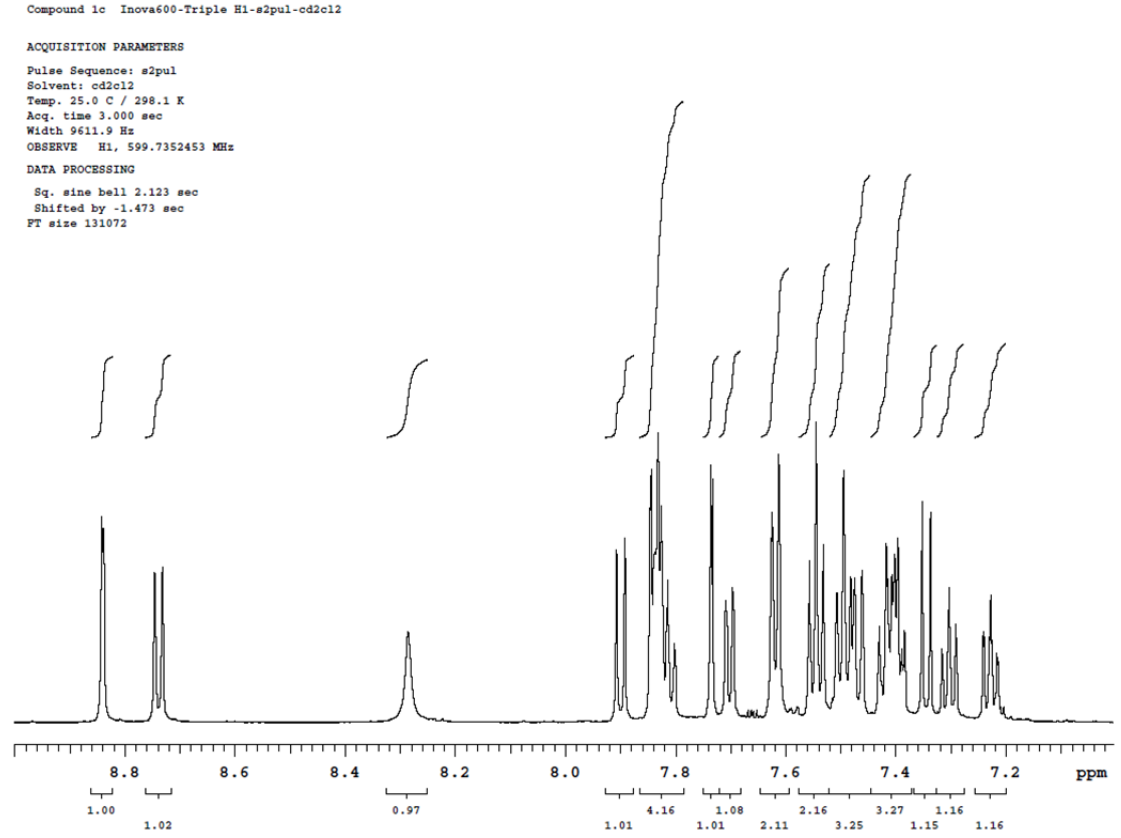
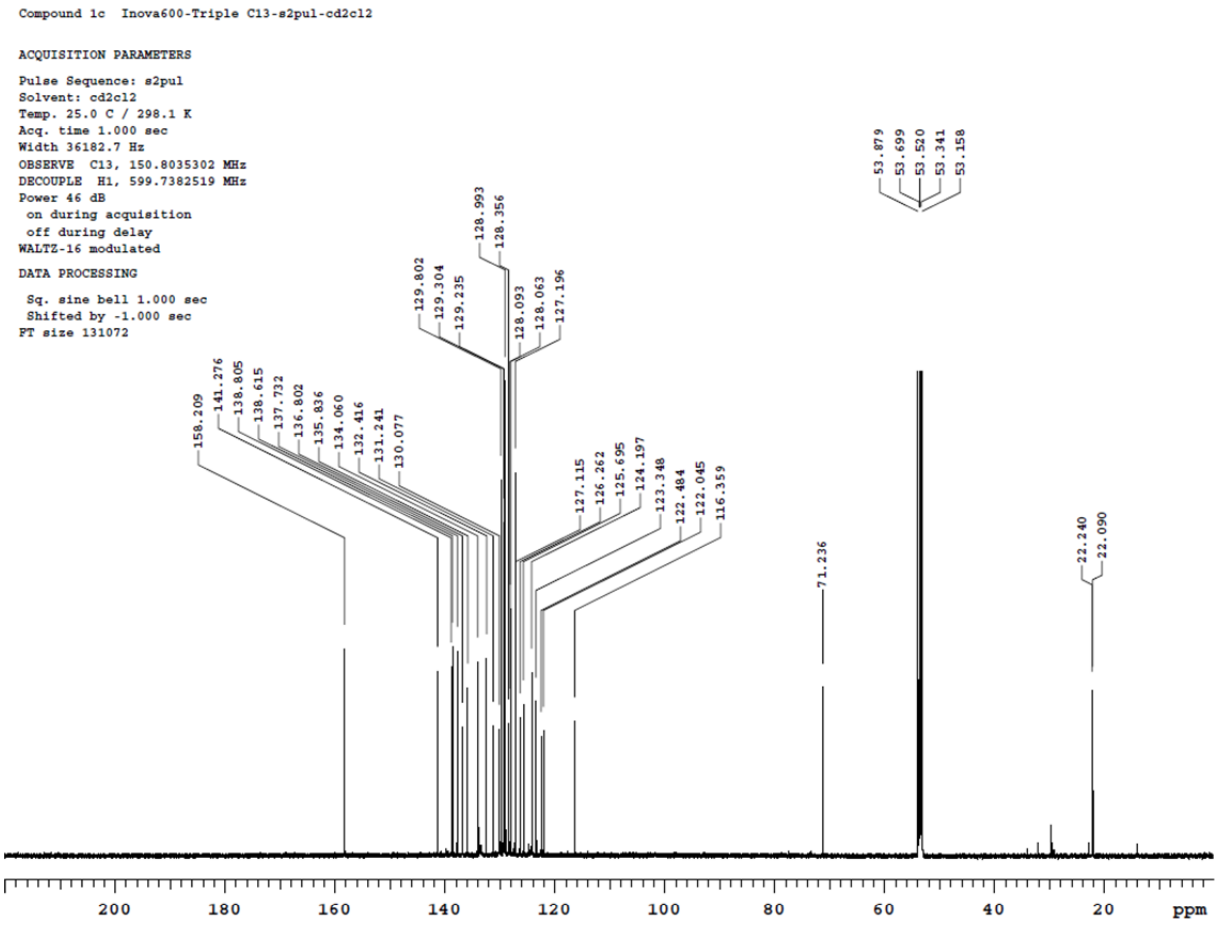


Figure S16. Up: ^{1}H NMR at 600 MHz in CD_2Cl_2 of compound **1c**. Bottom: Zoom of aromatic region.



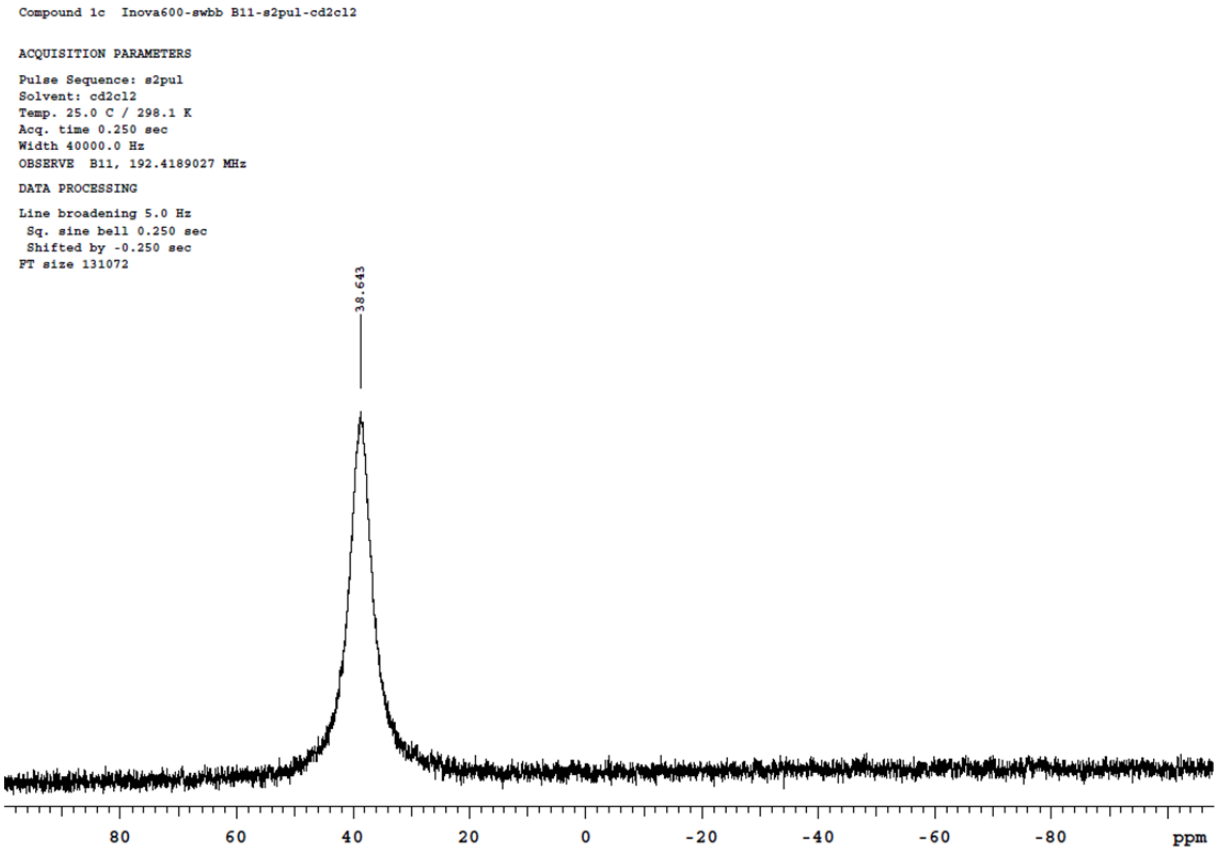


Figure S17. Compound **1c.** Up: ^{13}C NMR at 150.8 MHz, and bottom: ^{11}B NMR at 192.4 MHz in CD_2Cl_2.

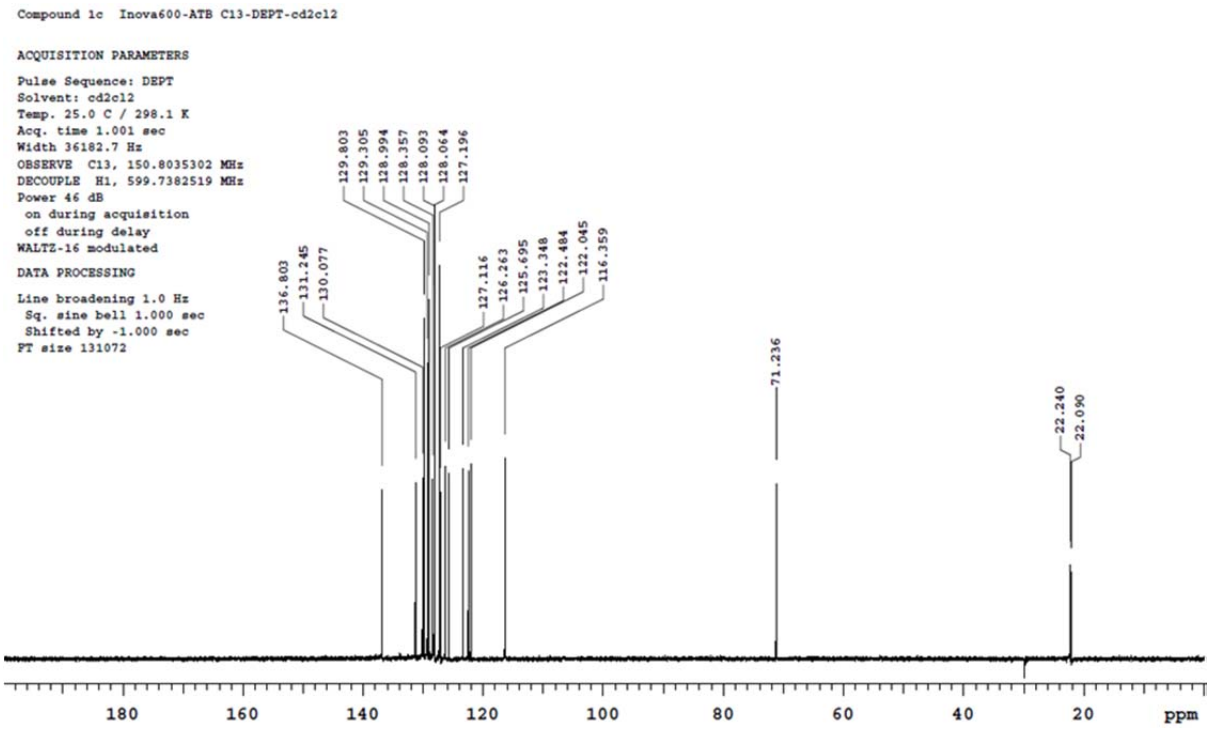
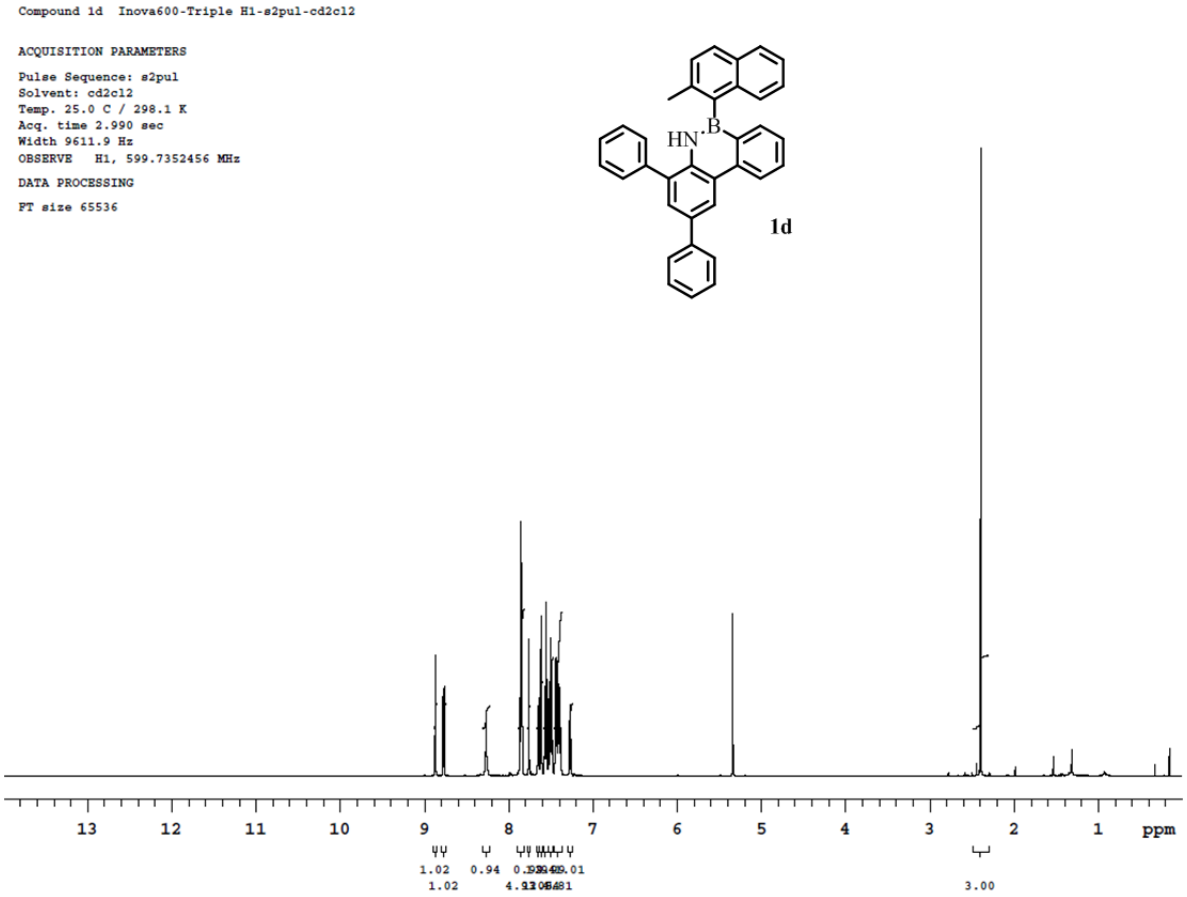


Figure S18. Compound **1c.** DEPT-135 at 150.8 MHz, in CD_2Cl_2.



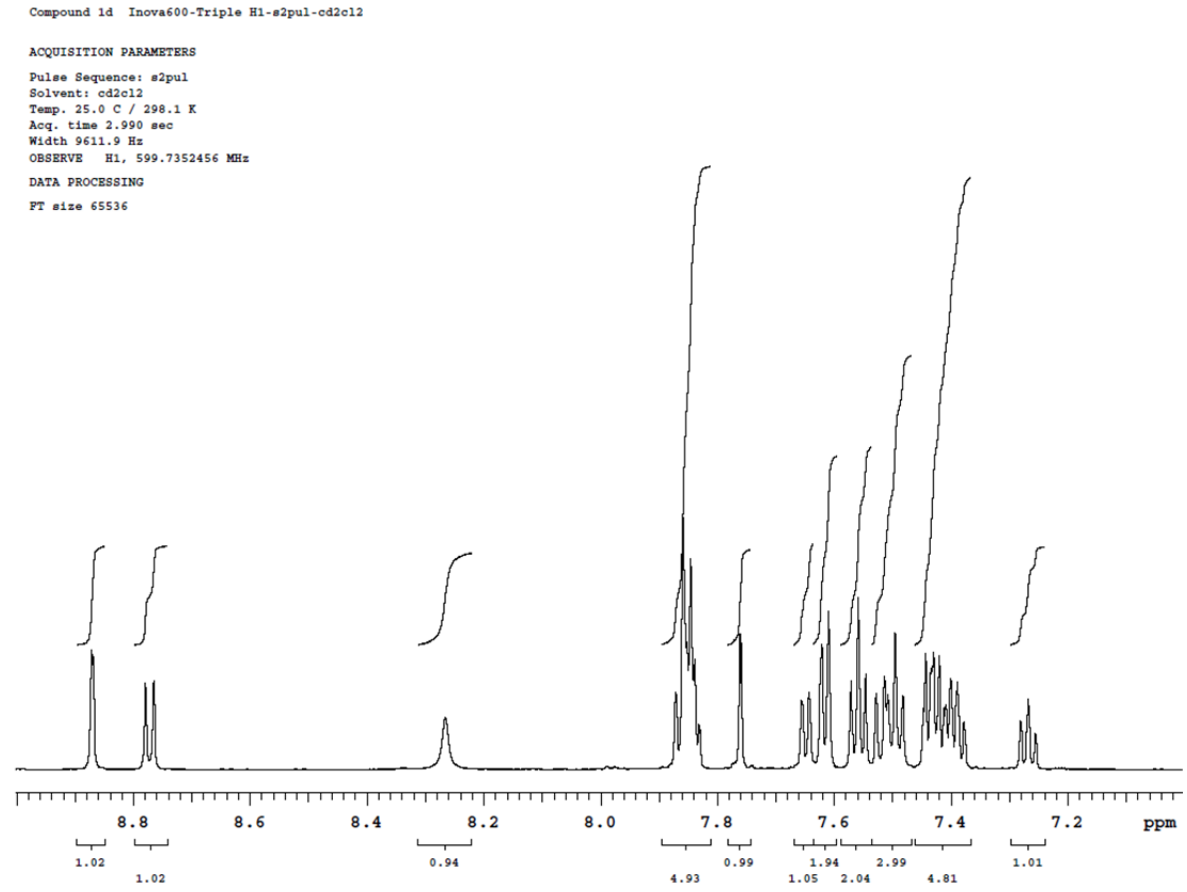
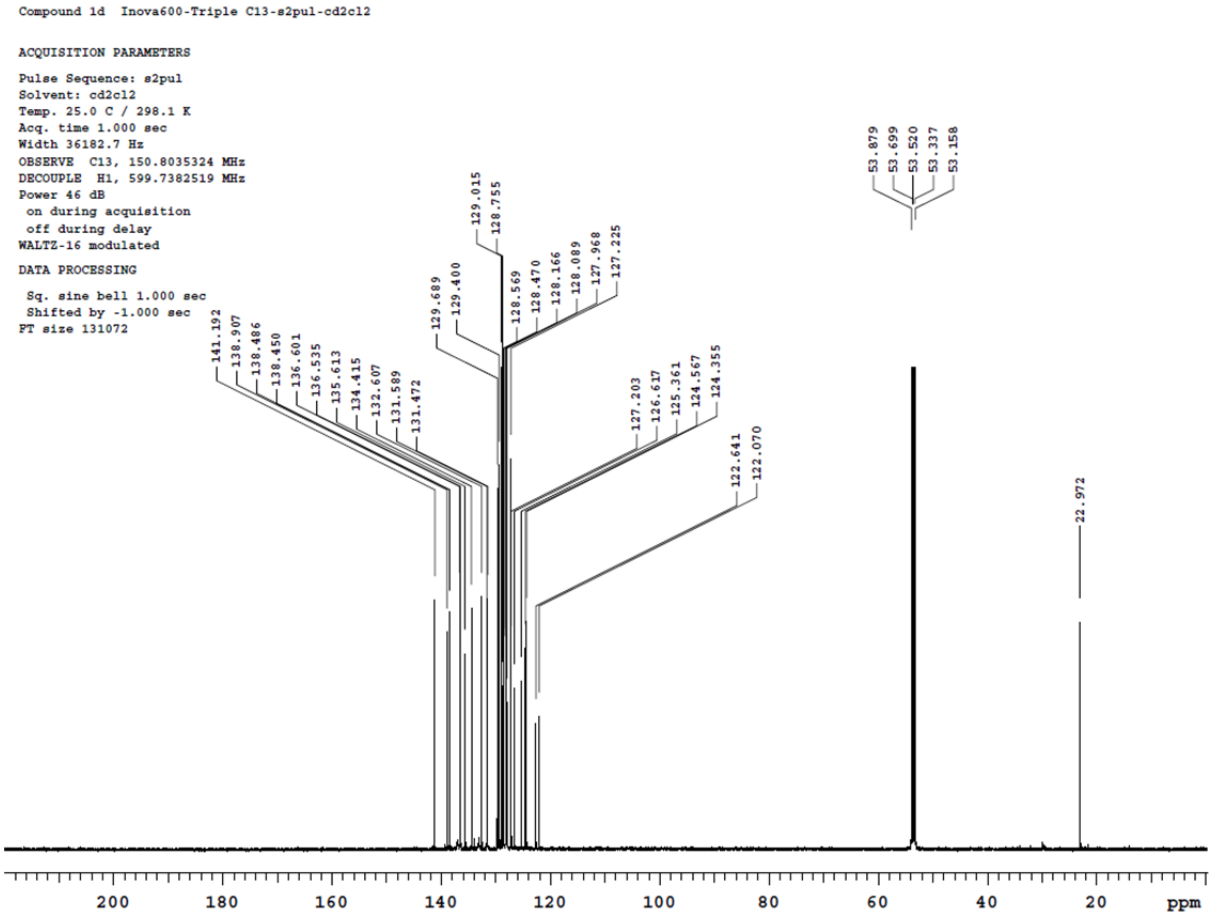


Figure S19. Up: ^{1}H NMR at 600 MHz in CD_2Cl_2 of compound **1d**. Bottom: Zoom of aromatic region.



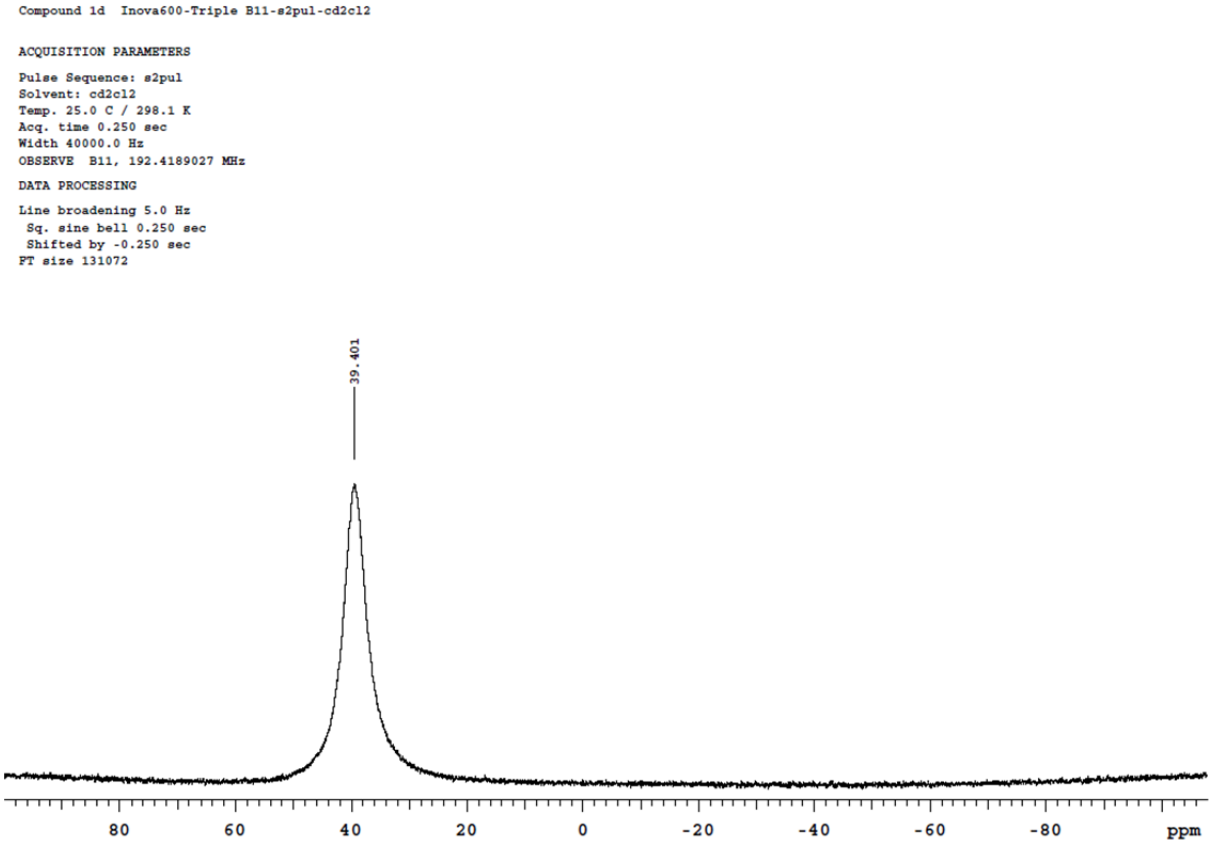


Figure S20. Compound **1d.** Up: ^{13}C NMR at 150.8 MHz, and bottom: ^{11}B NMR at 192.4 MHz in CD_2Cl_2.

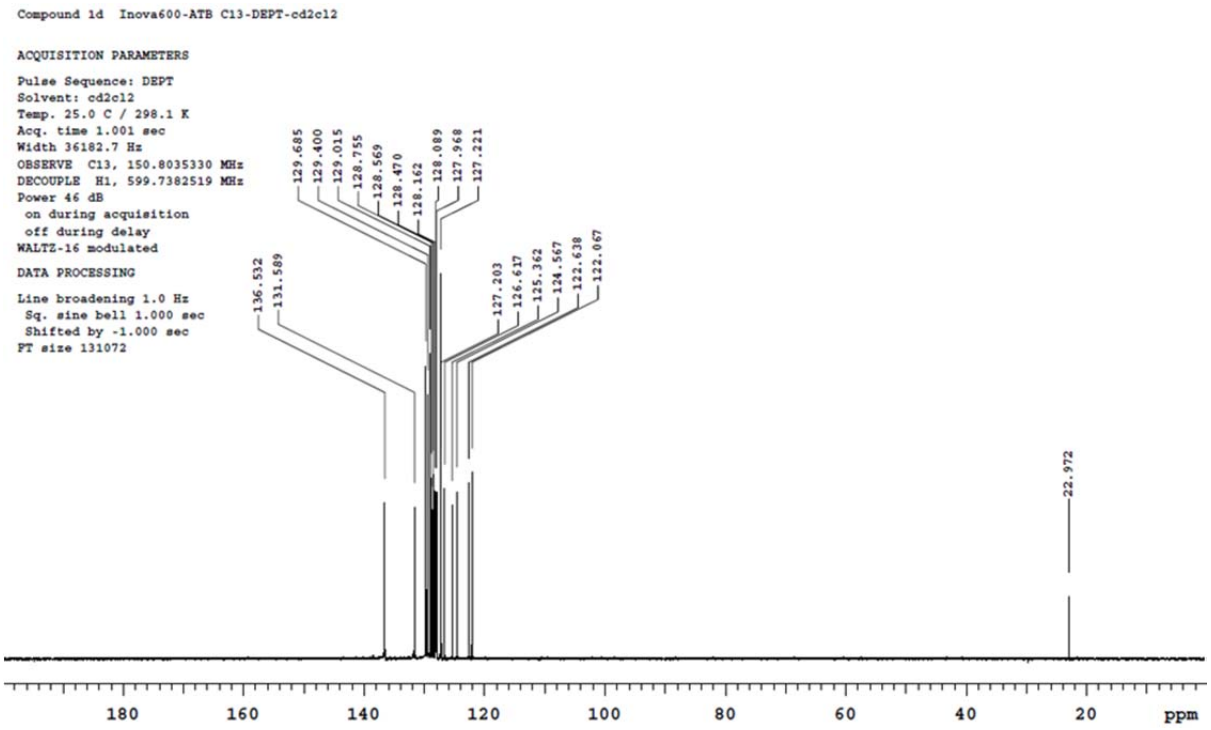
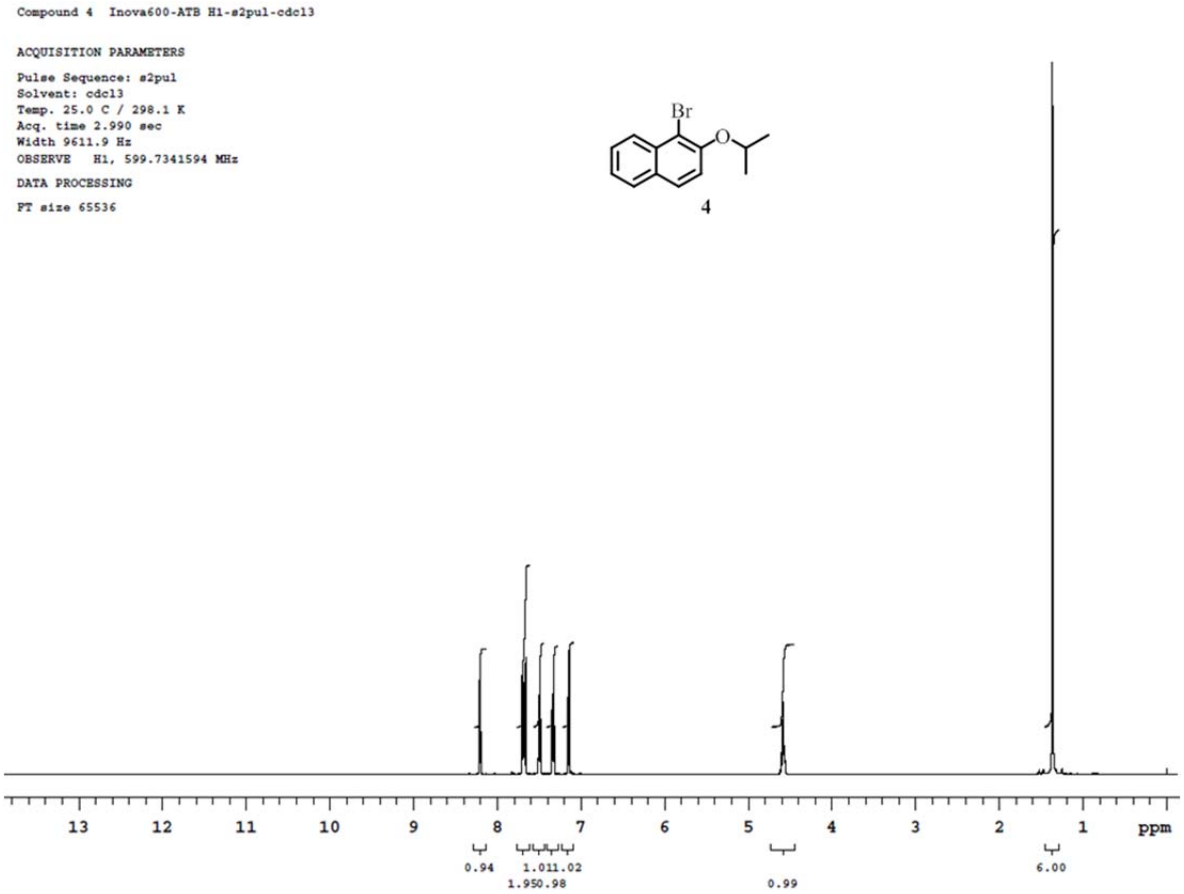


Figure S21. Compound **1d.** DEPT-135 at 150.8 MHz, in CD_2Cl_2.



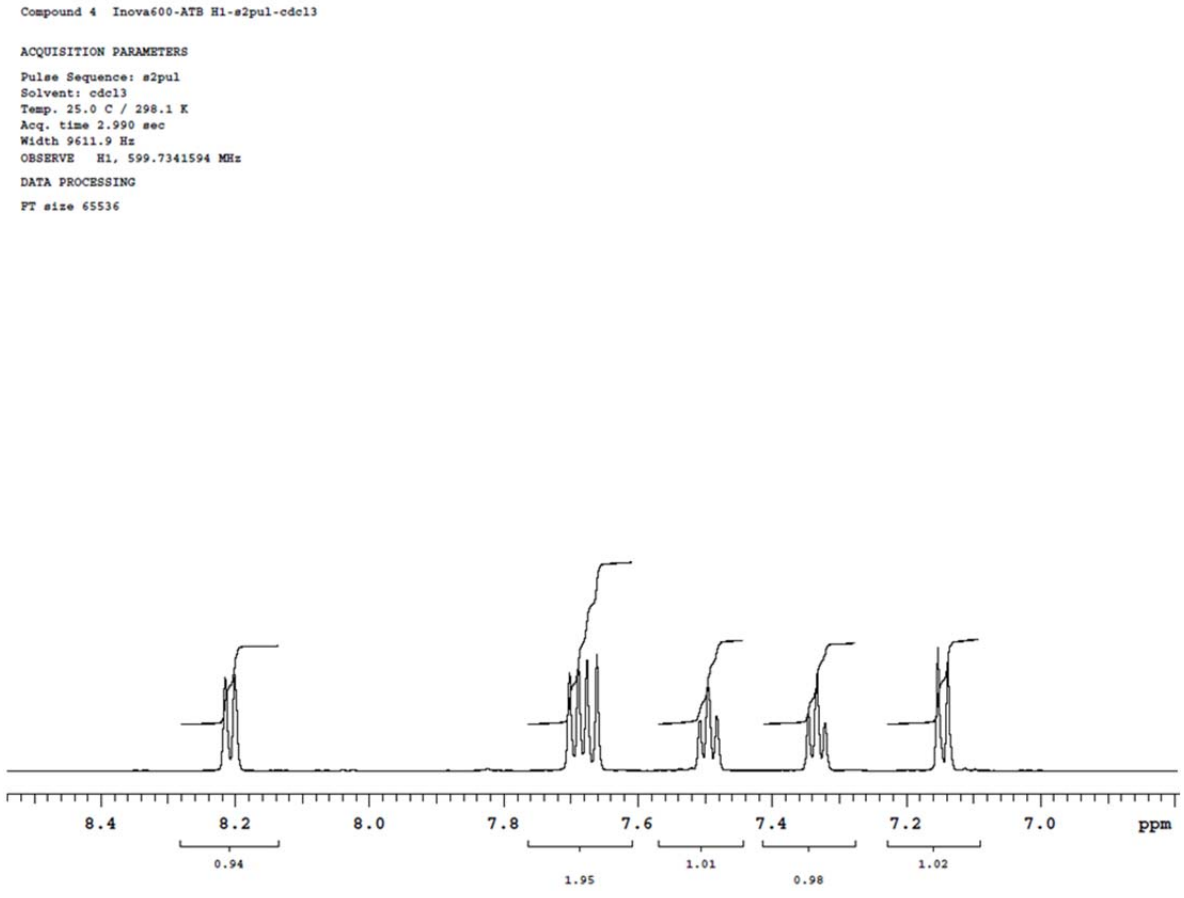


Figure S22. Up: ^{1}H NMR at 600 MHz in $CDCl_3$ of compound **4**. Bottom: Zoom of aromatic region.

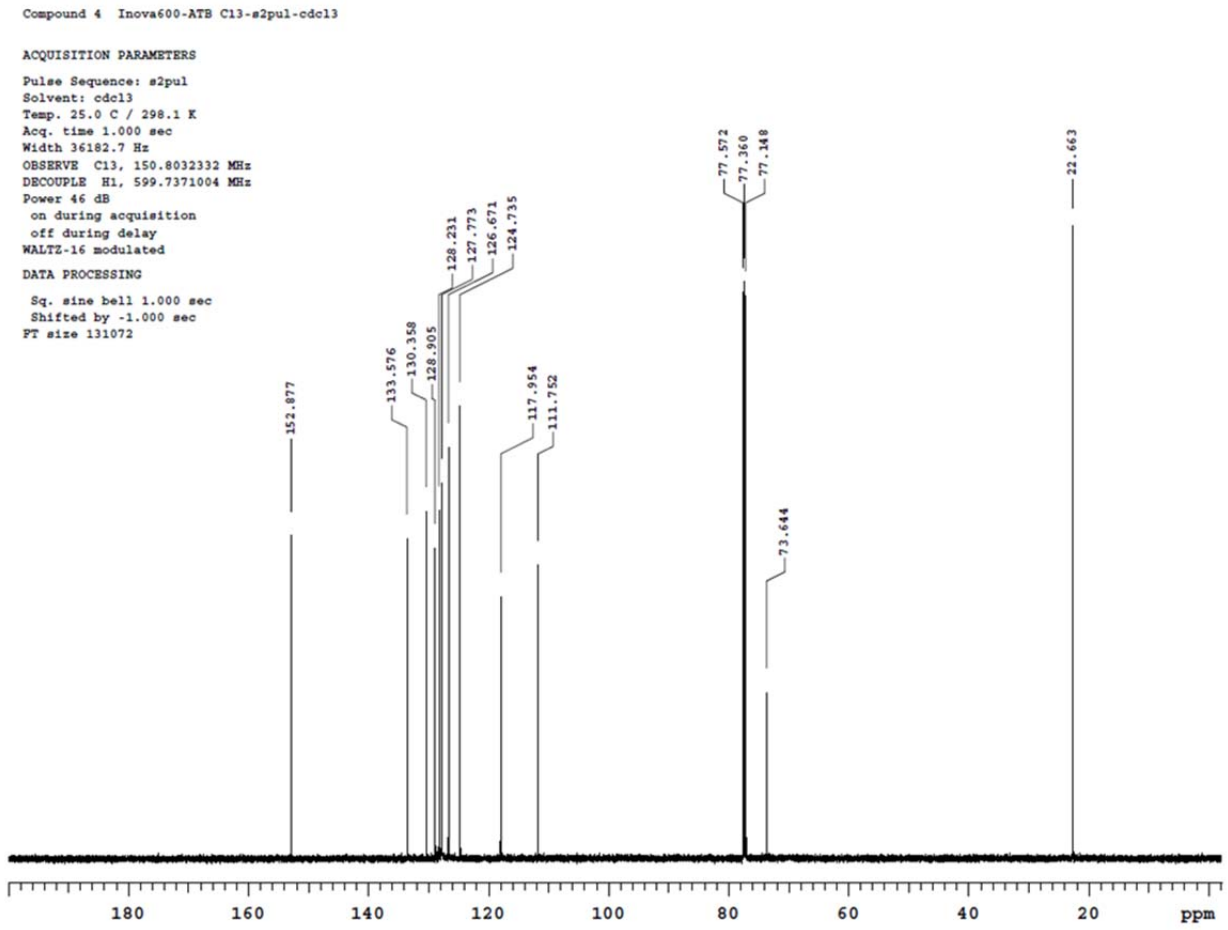


Figure S23. Compound **4.** ^{13}C NMR at 150.8 MHz in $CDCl_3$.

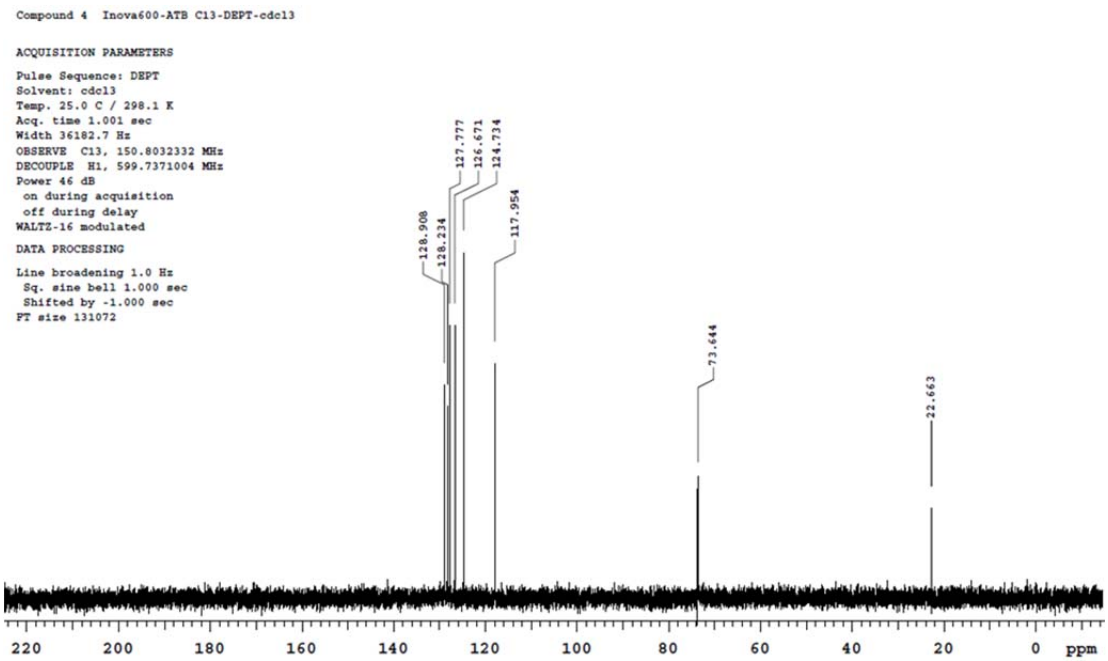


Figure S24. Compound **1d.** DEPT-135 at 150.8 MHz, in $CDCl_3$.

Compound 1a-GS1

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1275.47180965 A.U. after 1 cycles
Lowest frequency = 14.6671

Zero-point correction= 0.464064
(Hartree/Particle)
Thermal correction to Energy= 0.490136
Thermal correction to Enthalpy= 0.491080
Thermal correction to Gibbs Free Energy= 0.405365
Sum of electronic and zero-point Energies= -1275.007746
Sum of electronic and thermal Energies= -1274.981674
Sum of electronic and thermal Enthalpies= -1274.980730
Sum of electronic and thermal Free Energies= -1275.066445

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.383122	-3.364618	-0.039096
2	6	0	-1.844349	-4.642314	-0.035799
3	6	0	-0.451438	-4.793408	-0.051539
4	6	0	0.378001	-3.681614	-0.063692
5	6	0	-0.151588	-2.372402	-0.067098
6	6	0	-1.567380	-2.213811	-0.062606
7	6	0	0.723218	-1.184536	-0.067435
8	5	0	-2.171337	-0.792020	-0.055305
9	6	0	0.157754	0.118284	-0.082720
10	6	0	0.995389	1.265323	-0.100231
11	6	0	0.434591	2.648695	-0.127658
12	6	0	-0.394118	3.083650	-1.177413
13	6	0	-0.883060	4.390517	-1.208235
14	6	0	-0.549581	5.289266	-0.193768
15	6	0	0.277145	4.872790	0.851409
16	6	0	2.126339	-1.288188	-0.048858
17	6	0	2.968886	-0.177822	-0.039721
18	6	0	2.375784	1.096585	-0.066448
19	6	0	-3.710150	-0.444598	-0.075287
20	6	0	-4.352351	0.299712	0.944420
21	6	0	-5.718285	0.587357	0.830136
22	6	0	-6.461898	0.166326	-0.272740
23	6	0	-5.841757	-0.568578	-1.281619
24	6	0	-4.484285	-0.871804	-1.170516
25	6	0	-3.599162	0.787647	2.166688
26	1	0	-3.461744	-3.235548	-0.021018
27	1	0	-2.490791	-5.515717	-0.018471
28	1	0	-0.011566	-5.787702	-0.050440
29	1	0	1.449999	-3.844190	-0.071566
30	1	0	-0.636261	2.398459	-1.985963
31	1	0	-1.517257	4.707615	-2.031805
32	1	0	-0.929687	6.306897	-0.218323
33	1	0	0.541357	5.565311	1.646310
34	1	0	2.585678	-2.269106	-0.064888
35	1	0	3.005764	1.981183	-0.056337
36	1	0	-6.208754	1.148289	1.623257
37	1	0	-7.520655	0.404966	-0.336646
38	1	0	-6.409153	-0.908811	-2.144172

39	1	0	-4.009088	-1.453681	-1.957794
40	1	0	-4.291019	1.036091	2.978351
41	1	0	-2.896781	0.035923	2.542326
42	1	0	-3.014286	1.692957	1.956095
43	7	0	-1.224363	0.263798	-0.059982
44	1	0	-1.540141	1.227052	-0.064057
45	6	0	4.445634	-0.333079	-0.012328
46	6	0	5.052689	-1.343738	0.752920
47	6	0	5.277588	0.526571	-0.750089
48	6	0	6.438630	-1.492620	0.776026
49	1	0	4.431927	-2.001185	1.355541
50	6	0	6.663867	0.380825	-0.724399
51	1	0	4.831048	1.299598	-1.369509
52	6	0	7.251492	-0.630419	0.037866
53	1	0	6.884709	-2.277674	1.381230
54	1	0	7.285651	1.053456	-1.309628
55	1	0	8.331926	-0.744844	0.057180
56	6	0	0.762274	3.565476	0.884937
57	1	0	1.395806	3.241325	1.706076

Compound 1a-GS2

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1275.47184331 A.U. after 1 cycles
Lowest frequency = 16.1463

Zero-point correction= 0.463964
(Hartree/Particle)
Thermal correction to Energy= 0.490087
Thermal correction to Enthalpy= 0.491031
Thermal correction to Gibbs Free Energy= 0.405182
Sum of electronic and zero-point Energies= -1275.007880
Sum of electronic and thermal Energies= -1274.981756
Sum of electronic and thermal Enthalpies= -1274.980812
Sum of electronic and thermal Free Energies= -1275.066662

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.464668	-3.226562	-0.175223
2	6	0	-1.966822	-4.520627	-0.177600
3	6	0	-0.579953	-4.715285	-0.121925
4	6	0	0.283224	-3.630580	-0.072948
5	6	0	-0.205255	-2.305118	-0.069227
6	6	0	-1.613843	-2.103350	-0.112190
7	6	0	0.703998	-1.143773	-0.035485
8	5	0	-2.174410	-0.664945	-0.125843
9	6	0	0.178235	0.175899	-0.040896
10	6	0	1.049513	1.296756	-0.001580
11	6	0	0.532348	2.697248	0.002910
12	6	0	0.926306	3.599910	-0.998601
13	6	0	0.483132	4.922307	-0.985051
14	6	0	-0.366754	5.368536	0.028729
15	6	0	-0.765734	4.484135	1.032045
16	6	0	2.103054	-1.290501	-0.005575
17	6	0	2.978999	-0.206403	0.009428

18	6	0	2.424601	1.085451	0.010360
19	6	0	-3.695833	-0.253564	-0.217603
20	6	0	-4.609281	-0.415383	0.852846
21	6	0	-5.942152	-0.022024	0.684318
22	6	0	-6.392665	0.528387	-0.516919
23	6	0	-5.500826	0.700831	-1.573204
24	6	0	-4.168531	0.314858	-1.413808
25	6	0	-4.158627	-0.975250	2.186258
26	1	0	-3.537774	-3.061059	-0.230586
27	1	0	-2.639009	-5.373138	-0.226016
28	1	0	-0.171589	-5.722893	-0.122408
29	1	0	1.349061	-3.826997	-0.039043
30	1	0	1.577881	3.252869	-1.795913
31	1	0	0.798019	5.603381	-1.771318
32	1	0	-0.714450	6.397936	0.037496
33	1	0	-1.418722	4.824202	1.831419
34	1	0	2.530996	-2.285006	0.030770
35	1	0	3.081436	1.950297	0.017605
36	1	0	-6.638414	-0.144407	1.511557
37	1	0	-7.433932	0.822904	-0.621902
38	1	0	-5.836204	1.131691	-2.513199
39	1	0	-3.478431	0.451518	-2.244557
40	1	0	-4.994355	-1.042238	2.890365
41	1	0	-3.724173	-1.976149	2.084080
42	1	0	-3.388208	-0.343220	2.646612
43	7	0	-1.198682	0.363006	-0.104036
44	1	0	-1.488932	1.334393	-0.130290
45	6	0	4.450441	-0.406623	0.033025
46	6	0	5.282737	0.431225	0.795046
47	6	0	5.051896	-1.439066	-0.707122
48	6	0	6.664026	0.243492	0.816893
49	1	0	4.839259	1.220646	1.395706
50	6	0	6.432669	-1.629884	-0.682727
51	1	0	4.432096	-2.080429	-1.327787
52	6	0	7.245986	-0.788903	0.079029
53	1	0	7.285903	0.900018	1.420031
54	1	0	6.874854	-2.431067	-1.269358
55	1	0	8.322486	-0.935985	0.096685
56	6	0	-0.318977	3.162031	1.021135
57	1	0	-0.612446	2.487400	1.821488

Compound 1a TS0

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1275.45463740 A.U. after 1 cycles
Lowest frequency = -70.2220

Zero-point correction= 0.465067
(Hartree/Particle)
Thermal correction to Energy= 0.489799
Thermal correction to Enthalpy= 0.490743
Thermal correction to Gibbs Free Energy= 0.409738
Sum of electronic and zero-point Energies= -1274.989570
Sum of electronic and thermal Energies= -1274.964839
Sum of electronic and thermal Enthalpies= -1274.963894
Sum of electronic and thermal Free Energies= -1275.044899

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.269340	-3.472447	-0.721303
2	6	0	-1.662469	-4.705243	-0.909410
3	6	0	-0.278232	-4.818326	-0.757517
4	6	0	0.469018	-3.687747	-0.476249
5	6	0	-0.131744	-2.420753	-0.302782
6	6	0	-1.557790	-2.300790	-0.371610
7	6	0	0.722634	-1.231819	-0.139588
8	5	0	-2.205419	-0.887503	-0.109345
9	6	0	0.135711	0.052355	-0.219666
10	6	0	0.951132	1.215826	-0.238235
11	6	0	0.371149	2.580119	-0.404635
12	6	0	-0.387728	2.911854	-1.541307
13	6	0	-0.895178	4.200694	-1.711029
14	6	0	-0.652260	5.183432	-0.749076
15	6	0	0.103494	4.869065	0.381841
16	6	0	2.116756	-1.307839	0.031427
17	6	0	2.933929	-0.178970	0.081327
18	6	0	2.326175	1.078781	-0.077695
19	6	0	-3.709449	-0.506160	0.283510
20	6	0	-4.143046	0.776034	0.756694
21	6	0	-5.497067	0.991865	1.052307
22	6	0	-6.461862	-0.002416	0.920801
23	6	0	-6.060109	-1.267302	0.509260
24	6	0	-4.718267	-1.493361	0.213431
25	6	0	-3.238526	1.967463	1.018661
26	1	0	-3.333268	-3.421815	-0.901160
27	1	0	-2.260883	-5.570290	-1.182510
28	1	0	0.217532	-5.776119	-0.893091
29	1	0	1.547005	-3.788252	-0.430492
30	1	0	-0.562609	2.157084	-2.303712
31	1	0	-1.471778	4.438960	-2.600968
32	1	0	-1.046758	6.187190	-0.881530
33	1	0	0.296816	5.627330	1.136079
34	1	0	2.592424	-2.277430	0.113372
35	1	0	2.938095	1.975909	-0.062680
36	1	0	-5.798659	1.974431	1.408170
37	1	0	-7.501717	0.207244	1.158310
38	1	0	-6.777066	-2.079805	0.424462
39	1	0	-4.452673	-2.501131	-0.060473
40	1	0	-3.781574	2.731479	1.583018
41	1	0	-2.354458	1.702611	1.607556
42	1	0	-2.897998	2.459813	0.097270
43	7	0	-1.247171	0.166177	-0.206313
44	1	0	-1.554652	1.126516	-0.174127
45	6	0	4.400886	-0.300328	0.277548
46	6	0	4.935591	-1.259912	1.154487
47	6	0	5.295708	0.540647	-0.406289
48	6	0	6.312628	-1.377449	1.337500
49	1	0	4.262447	-1.901134	1.717067
50	6	0	6.672723	0.426278	-0.220831
51	1	0	4.908511	1.273141	-1.109288
52	6	0	7.188440	-0.534229	0.651217
53	1	0	6.701323	-2.122827	2.026638
54	1	0	7.344661	1.083314	-0.767071
55	1	0	8.261760	-0.624200	0.795080

56	6	0	0.609145	3.580030	0.552556
57	1	0	1.188488	3.336147	1.438938

Compound 1a TS180

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1275.44683719 A.U. after 1 cycles
Lowest frequency = -63.6619

Zero-point correction= 0.465176
(Hartree/Particle)
Thermal correction to Energy= 0.489865
Thermal correction to Enthalpy= 0.490809
Thermal correction to Gibbs Free Energy= 0.409760
Sum of electronic and zero-point Energies= -1274.981661
Sum of electronic and thermal Energies= -1274.956972
Sum of electronic and thermal Enthalpies= -1274.956028
Sum of electronic and thermal Free Energies= -1275.037077

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.788153	-4.538996	-1.077025
2	6	0	-0.411971	-4.711818	-0.911468
3	6	0	0.373818	-3.622858	-0.572680
4	6	0	-0.181857	-2.343610	-0.351929
5	6	0	-1.603918	-2.172495	-0.415894
6	6	0	0.713280	-1.190756	-0.164636
7	5	0	-2.202992	-0.744969	-0.131299
8	6	0	0.172923	0.110680	-0.279457
9	6	0	1.026558	1.247058	-0.286762
10	6	0	0.492961	2.629243	-0.456172
11	6	0	-0.277901	2.983216	-1.578476
12	6	0	-0.743711	4.288222	-1.744226
13	6	0	-0.445342	5.266549	-0.794528
14	6	0	0.321964	4.930787	0.322707
15	6	0	2.097653	-1.315182	0.045277
16	6	0	2.951714	-0.213661	0.100106
17	6	0	2.391710	1.062203	-0.089536
18	6	0	-3.631600	-0.178281	0.373600
19	6	0	-4.891046	-0.835650	0.535884
20	6	0	-6.012804	-0.113012	0.975726
21	6	0	-5.963123	1.238048	1.297346
22	6	0	-4.738865	1.890126	1.212318
23	6	0	-3.623324	1.184601	0.773956
24	1	0	-2.413658	-5.365755	-1.403281
25	1	0	0.050094	-5.680098	-1.086251
26	1	0	1.448063	-3.760715	-0.528945
27	1	0	-0.492516	2.233774	-2.336074
28	1	0	-1.332025	4.541209	-2.622259
29	1	0	-0.807047	6.282925	-0.924311
30	1	0	0.557084	5.685152	1.068977
31	1	0	2.533487	-2.300896	0.156698
32	1	0	3.034295	1.937410	-0.064921
33	1	0	-6.957109	-0.642515	1.077597
34	1	0	-6.856496	1.757704	1.633910

35	1	0	-4.639887	2.934705	1.495408
36	1	0	-2.693233	1.740279	0.792965
37	7	0	-1.203264	0.267486	-0.301688
38	1	0	-1.476288	1.240486	-0.323341
39	6	0	4.408069	-0.381507	0.336456
40	6	0	4.887163	-1.346014	1.239782
41	6	0	5.348314	0.419015	-0.334912
42	6	0	6.254238	-1.507173	1.460333
43	1	0	4.178368	-1.956272	1.792950
44	6	0	6.715423	0.261096	-0.111891
45	1	0	5.004370	1.153947	-1.057586
46	6	0	7.175615	-0.703694	0.786105
47	1	0	6.599518	-2.255364	2.169276
48	1	0	7.423128	0.887343	-0.649074
49	1	0	8.241204	-0.827656	0.959240
50	6	0	0.783780	3.625641	0.491204
51	1	0	1.368906	3.365298	1.368958
52	6	0	-5.151804	-2.308201	0.304039
53	1	0	-5.202564	-2.557519	-0.763033
54	1	0	-4.389950	-2.940591	0.764813
55	1	0	-6.117125	-2.588595	0.736719
56	6	0	-2.352221	-3.294949	-0.831878
57	1	0	-3.408058	-3.183581	-1.010345

Compound 1b GS1

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1314.78523850 A.U. after 1 cycles
Lowest frequency = 15.4713

Zero-point correction= 0.492964
(Hartree/Particle)
Thermal correction to Energy= 0.520266
Thermal correction to Enthalpy= 0.521210
Thermal correction to Gibbs Free Energy= 0.432758
Sum of electronic and zero-point Energies= -1314.292274
Sum of electronic and thermal Energies= -1314.264972
Sum of electronic and thermal Enthalpies= -1314.264028
Sum of electronic and thermal Free Energies= -1314.352481

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.311810	-3.248670	-0.320669
2	6	0	-1.807832	-4.540255	-0.305216
3	6	0	-0.422132	-4.728051	-0.212256
4	6	0	0.434213	-3.638939	-0.144105
5	6	0	-0.060292	-2.315901	-0.158423
6	6	0	-1.468402	-2.120860	-0.239938
7	6	0	0.842982	-1.150600	-0.105237
8	5	0	-2.034917	-0.684477	-0.277186
9	6	0	0.312054	0.166589	-0.130219
10	6	0	1.177071	1.291391	-0.072989
11	6	0	0.653313	2.689464	-0.089266
12	6	0	1.062036	3.586440	-1.089893
13	6	0	0.611899	4.906590	-1.095042

14	6	0	-0.259585	5.355969	-0.101202
15	6	0	-0.673267	4.477200	0.901140
16	6	0	2.241375	-1.290996	-0.037334
17	6	0	3.111954	-0.202988	-0.003837
18	6	0	2.552221	1.086448	-0.023618
19	6	0	-3.552509	-0.277211	-0.435804
20	6	0	-4.529951	-0.456386	0.572855
21	6	0	-5.854829	-0.073719	0.322961
22	6	0	-6.234502	0.484945	-0.897196
23	6	0	-5.278258	0.676410	-1.893609
24	6	0	-3.956294	0.299868	-1.654979
25	6	0	-4.165729	-0.985499	1.948384
26	1	0	-3.383983	-3.088855	-0.401607
27	1	0	-2.474618	-5.396065	-0.367792
28	1	0	-0.009041	-5.733636	-0.198223
29	1	0	1.499621	-3.830071	-0.080305
30	1	0	1.730857	3.236760	-1.871629
31	1	0	0.938519	5.583416	-1.880189
32	1	0	-0.612570	6.383594	-0.106990
33	1	0	-1.343225	4.819888	1.685187
34	1	0	2.672559	-2.283398	0.014613
35	1	0	3.204833	1.954283	-0.003338
36	1	0	-6.601153	-0.215758	1.102615
37	1	0	-7.270418	0.768025	-1.066889
38	1	0	-5.558482	1.111103	-2.849779
39	1	0	-3.218196	0.445985	-2.441692
40	1	0	-5.039206	-1.483230	2.388725
41	1	0	-3.382030	-1.746910	1.867158
42	7	0	-1.063518	0.347526	-0.230898
43	1	0	-1.356486	1.317657	-0.271656
44	6	0	4.583089	-0.396631	0.059710
45	6	0	5.391255	0.448327	0.839635
46	6	0	5.208398	-1.429743	-0.659436
47	6	0	6.772275	0.266791	0.898969
48	1	0	4.928600	1.238502	1.424639
49	6	0	6.588843	-1.614354	-0.597553
50	1	0	4.608065	-2.076650	-1.293343
51	6	0	7.378037	-0.766354	0.181591
52	1	0	7.375085	0.928776	1.515352
53	1	0	7.049861	-2.416216	-1.168550
54	1	0	8.454311	-0.908601	0.228475
55	6	0	-0.219723	3.157391	0.908875
56	1	0	-0.524300	2.487552	1.709227
57	6	0	-3.688140	0.122775	2.904936
58	1	0	-4.460338	0.889566	3.035498
59	1	0	-3.444708	-0.288844	3.891423
60	1	0	-2.790905	0.616183	2.513880

Compound 1b GS2

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1314.78509475 A.U. after 1 cycles
Lowest frequency = 14.8499

Zero-point correction= 0.492991
(Hartree/Particle)
Thermal correction to Energy= 0.520309
Thermal correction to Enthalpy= 0.521253

Thermal correction to Gibbs Free Energy= 0.432440
Sum of electronic and zero-point Energies= -1314.292103
Sum of electronic and thermal Energies= -1314.264786
Sum of electronic and thermal Enthalpies= -1314.263841
Sum of electronic and thermal Free Energies= -1314.352654

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.311171	-3.262321	-0.344383
2	6	0	-1.800657	-4.551467	-0.367308
3	6	0	-0.411628	-4.733516	-0.336646
4	6	0	0.442123	-3.641461	-0.280062
5	6	0	-0.058365	-2.321165	-0.255448
6	6	0	-1.469454	-2.131260	-0.293867
7	6	0	0.840100	-1.152958	-0.188748
8	5	0	-2.043931	-0.698496	-0.260070
9	6	0	0.303234	0.162089	-0.190110
10	6	0	1.165078	1.290256	-0.148914
11	6	0	0.635921	2.686160	-0.161358
12	6	0	-0.149182	3.163794	-1.225899
13	6	0	-0.607963	4.481768	-1.241016
14	6	0	-0.287021	5.349191	-0.195727
15	6	0	0.496822	4.890195	0.864521
16	6	0	2.238962	-1.288364	-0.120684
17	6	0	3.103966	-0.197560	-0.052364
18	6	0	2.539479	1.089853	-0.069533
19	6	0	-3.576141	-0.321928	-0.324335
20	6	0	-4.286034	0.281762	0.741995
21	6	0	-5.635276	0.618591	0.566840
22	6	0	-6.298799	0.371566	-0.634477
23	6	0	-5.612788	-0.232050	-1.687688
24	6	0	-4.270759	-0.575367	-1.522806
25	6	0	-3.646780	0.511190	2.100444
26	1	0	-3.386501	-3.107351	-0.366904
27	1	0	-2.465715	-5.409998	-0.407360
28	1	0	0.006193	-5.737090	-0.355675
29	1	0	1.509949	-3.828432	-0.257406
30	1	0	-0.380690	2.503087	-2.057596
31	1	0	-1.208777	4.832002	-2.076102
32	1	0	-0.643846	6.375435	-0.207958
33	1	0	0.750756	5.558039	1.683513
34	1	0	2.677344	-2.278703	-0.143674
35	1	0	3.187354	1.959745	-0.014643
36	1	0	-6.174099	1.083599	1.390497
37	1	0	-7.344384	0.648244	-0.745203
38	1	0	-6.116265	-0.432815	-2.630016
39	1	0	-3.743244	-1.045863	-2.350514
40	1	0	-2.592059	0.784988	1.986057
41	1	0	-4.137425	1.360275	2.593014
42	7	0	-1.076374	0.337627	-0.210241
43	1	0	-1.373673	1.306993	-0.197041
44	6	0	4.575013	-0.386113	0.026412
45	6	0	5.130912	-1.427787	0.788904
46	6	0	5.452361	0.472191	-0.658398
47	6	0	6.511523	-1.607663	0.860401
48	1	0	4.473814	-2.085498	1.351396

49	6	0	6.833266	0.295322	-0.584286
50	1	0	5.046123	1.269352	-1.274962
51	6	0	7.369909	-0.746352	0.174580
52	1	0	6.917578	-2.416438	1.462535
53	1	0	7.490970	0.967715	-1.129123
54	1	0	8.446164	-0.884976	0.231676
55	6	0	0.951610	3.571769	0.882262
56	1	0	1.551245	3.214494	1.715032
57	6	0	-3.741360	-0.723715	3.015886
58	1	0	-3.283114	-0.523460	3.991517
59	1	0	-4.786508	-1.008974	3.181682
60	1	0	-3.228335	-1.583184	2.570177

Compound 1b GS3

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1314.78525069 A.U. after 1 cycles
Lowest frequency = 16.0154

Zero-point correction= 0.492968
(Hartree/Particle)
Thermal correction to Energy= 0.520269
Thermal correction to Enthalpy= 0.521213
Thermal correction to Gibbs Free Energy= 0.432751
Sum of electronic and zero-point Energies= -1314.292283
Sum of electronic and thermal Energies= -1314.264982
Sum of electronic and thermal Enthalpies= -1314.264037
Sum of electronic and thermal Free Energies= -1314.352499

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.334657	-3.212502	-0.519176
2	6	0	-1.833471	-4.501054	-0.624194
3	6	0	-0.445760	-4.695035	-0.596951
4	6	0	0.415225	-3.614845	-0.469519
5	6	0	-0.076501	-2.295371	-0.359372
6	6	0	-1.485856	-2.094432	-0.380952
7	6	0	0.830350	-1.138035	-0.237859
8	5	0	-2.049676	-0.660066	-0.281560
9	6	0	0.304339	0.180988	-0.204535
10	6	0	1.174880	1.299727	-0.119374
11	6	0	0.658085	2.700012	-0.094941
12	6	0	-0.115041	3.215241	-1.150536
13	6	0	-0.561020	4.537469	-1.131398
14	6	0	-0.239392	5.371683	-0.059627
15	6	0	0.532321	4.875131	0.992525
16	6	0	2.226795	-1.288044	-0.155032
17	6	0	3.099979	-0.207303	-0.043395
18	6	0	2.546696	1.084903	-0.030545
19	6	0	-3.573582	-0.247086	-0.314272
20	6	0	-4.483453	-0.497633	0.741254
21	6	0	-5.821109	-0.102469	0.604768
22	6	0	-6.278822	0.536303	-0.547421
23	6	0	-5.389635	0.796822	-1.589217
24	6	0	-4.055468	0.409056	-1.462934

25	6	0	-4.030751	-1.120263	2.049563
26	1	0	-3.408648	-3.046969	-0.548073
27	1	0	-2.504064	-5.349459	-0.731186
28	1	0	-0.034849	-5.697991	-0.682264
29	1	0	1.481972	-3.809292	-0.464719
30	1	0	-0.347130	2.580143	-2.001740
31	1	0	-1.152458	4.917335	-1.960230
32	1	0	-0.586556	6.401195	-0.044976
33	1	0	0.786320	5.516770	1.832161
34	1	0	2.656556	-2.281534	-0.197495
35	1	0	3.201181	1.947035	0.057947
36	1	0	-6.515185	-0.299129	1.419958
37	1	0	-7.323133	0.827365	-0.629528
38	1	0	-5.731449	1.293284	-2.493938
39	1	0	-3.370346	0.608739	-2.285155
40	1	0	-4.876524	-1.643637	2.513614
41	1	0	-3.261301	-1.877688	1.862358
42	7	0	-1.074326	0.367779	-0.223152
43	1	0	-1.366421	1.336613	-0.154851
44	6	0	4.568135	-0.411108	0.050446
45	6	0	5.104258	-1.479004	0.790480
46	6	0	5.462310	0.458588	-0.597178
47	6	0	6.482143	-1.673033	0.876109
48	1	0	4.433709	-2.146660	1.324675
49	6	0	6.840482	0.267447	-0.508880
50	1	0	5.071600	1.276589	-1.196234
51	6	0	7.357436	-0.800144	0.227295
52	1	0	6.872751	-2.502194	1.460468
53	1	0	7.511534	0.949248	-1.024986
54	1	0	8.431560	-0.949858	0.295443
55	6	0	0.974669	3.552505	0.975641
56	1	0	1.564719	3.165881	1.802104
57	6	0	-3.478922	-0.081767	3.043915
58	1	0	-3.174062	-0.561382	3.981420
59	1	0	-2.605534	0.433360	2.628458
60	1	0	-4.233589	0.677647	3.278516

Compound 1b GS4

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1314.78493403 A.U. after 1 cycles
Lowest frequency = 14.8380

Zero-point correction= 0.492925
(Hartree/Particle)
Thermal correction to Energy= 0.520255
Thermal correction to Enthalpy= 0.521199
Thermal correction to Gibbs Free Energy= 0.432374
Sum of electronic and zero-point Energies= -1314.292009
Sum of electronic and thermal Energies= -1314.264679
Sum of electronic and thermal Enthalpies= -1314.263735
Sum of electronic and thermal Free Energies= -1314.352560

Standard orientation:

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

1	6	0	-2.298474	-3.273260	-0.146545
2	6	0	-1.790544	-4.559884	-0.047763
3	6	0	-0.404167	-4.737995	0.050954
4	6	0	0.449773	-3.644583	0.049256
5	6	0	-0.048113	-2.326992	-0.051915
6	6	0	-1.456549	-2.141255	-0.152339
7	6	0	0.849892	-1.156688	-0.053039
8	5	0	-2.029038	-0.710880	-0.253652
9	6	0	0.311707	0.156654	-0.109292
10	6	0	1.172071	1.286377	-0.095325
11	6	0	0.640414	2.680708	-0.145622
12	6	0	1.021271	3.546631	-1.183808
13	6	0	0.563221	4.863581	-1.221603
14	6	0	-0.288168	5.340538	-0.223259
15	6	0	-0.673915	4.492773	0.816294
16	6	0	2.249846	-1.288621	-0.003338
17	6	0	3.115388	-0.196159	-0.012807
18	6	0	2.548734	1.089628	-0.058765
19	6	0	-3.554110	-0.347949	-0.445969
20	6	0	-4.339411	0.310280	0.531237
21	6	0	-5.674892	0.624458	0.244409
22	6	0	-6.252186	0.301838	-0.983161
23	6	0	-5.491701	-0.356047	-1.949119
24	6	0	-4.162751	-0.677315	-1.672312
25	6	0	-3.796751	0.624137	1.914460
26	1	0	-3.371771	-3.121079	-0.222640
27	1	0	-2.455680	-5.419277	-0.044079
28	1	0	0.011311	-5.739405	0.132526
29	1	0	1.515134	-3.828085	0.133561
30	1	0	1.674422	3.175105	-1.968686
31	1	0	0.867905	5.516130	-2.035564
32	1	0	-0.647174	6.365620	-0.254316
33	1	0	-1.327710	4.857645	1.604004
34	1	0	2.686754	-2.277595	0.064136
35	1	0	3.196987	1.960870	-0.072550
36	1	0	-6.271830	1.131783	1.000269
37	1	0	-7.288842	0.562302	-1.181978
38	1	0	-5.927572	-0.615708	-2.910530
39	1	0	-3.576866	-1.190809	-2.432331
40	1	0	-2.736903	0.896629	1.854851
41	1	0	-4.321819	1.498324	2.320198
42	7	0	-1.065106	0.328943	-0.209962
43	1	0	-1.358146	1.295532	-0.301143
44	6	0	4.588346	-0.381048	0.031767
45	6	0	5.404501	0.488118	0.775950
46	6	0	5.207419	-1.429728	-0.670033
47	6	0	6.787234	0.314895	0.817650
48	1	0	4.947128	1.291264	1.347296
49	6	0	6.589638	-1.605925	-0.625723
50	1	0	4.600405	-2.096035	-1.276908
51	6	0	7.386802	-0.733868	0.117961
52	1	0	7.396414	0.995834	1.406512
53	1	0	7.045642	-2.420314	-1.182850
54	1	0	8.464425	-0.869628	0.151103
55	6	0	-0.212682	3.176229	0.856320
56	1	0	-0.494112	2.531020	1.684839
57	6	0	-3.950925	-0.553798	2.894476
58	1	0	-3.405972	-1.434948	2.538102
59	1	0	-3.562336	-0.292394	3.885819

60	1	0	-5.004370	-0.835372	3.004361

Compound 1b TS0

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1314.76415541 A.U. after 1 cycles
Lowest frequency = -58.9230

Zero-point correction= 0.493933
(Hartree/Particle)
Thermal correction to Energy= 0.520002
Thermal correction to Enthalpy= 0.520946
Thermal correction to Gibbs Free Energy= 0.436984
Sum of electronic and zero-point Energies= -1314.270223
Sum of electronic and thermal Energies= -1314.244154
Sum of electronic and thermal Enthalpies= -1314.243209
Sum of electronic and thermal Free Energies= -1314.327171

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.895165	-3.730855	0.713795
2	6	0	1.209681	-4.929042	0.848603
3	6	0	-0.174661	-4.952149	0.663031
4	6	0	-0.844002	-3.768606	0.404919
5	6	0	-0.162846	-2.536457	0.286324
6	6	0	1.266626	-2.506334	0.385687
7	6	0	-0.941473	-1.293266	0.150858
8	5	0	2.003936	-1.124591	0.183537
9	6	0	-0.281015	-0.051852	0.297138
10	6	0	-1.024455	1.158209	0.341203
11	6	0	-0.364552	2.477410	0.564408
12	6	0	0.385779	2.726788	1.727408
13	6	0	0.973070	3.973710	1.945897
14	6	0	0.819860	4.996430	1.007472
15	6	0	0.072855	4.764459	-0.149166
16	6	0	-2.332748	-1.277403	-0.055339
17	6	0	-3.079003	-0.099474	-0.077885
18	6	0	-2.400784	1.111908	0.144302
19	6	0	3.535452	-0.822869	-0.181333
20	6	0	4.071309	0.440457	-0.613513
21	6	0	5.444804	0.559492	-0.865264
22	6	0	6.329742	-0.508879	-0.736898
23	6	0	5.828819	-1.751385	-0.375490
24	6	0	4.466401	-1.882900	-0.117991
25	6	0	3.214780	1.683010	-0.858431
26	1	0	2.954891	-3.753411	0.921449
27	1	0	1.747871	-5.837002	1.107373
28	1	0	-0.731191	-5.881163	0.756381
29	1	0	-1.924962	-3.799508	0.335494
30	1	0	0.491844	1.941297	2.471247
31	1	0	1.542096	4.148425	2.855220
32	1	0	1.276158	5.967688	1.178152
33	1	0	-0.052905	5.554968	-0.884406
34	1	0	-2.863371	-2.212167	-0.188686
35	1	0	-2.956781	2.044852	0.148694

36	1	0	5.843291	1.515774	-1.184023
37	1	0	7.388402	-0.367298	-0.939795
38	1	0	6.481374	-2.617145	-0.297955
39	1	0	4.119553	-2.874793	0.118346
40	1	0	2.310679	1.385773	-1.401272
41	1	0	2.877654	2.099636	0.102910
42	7	0	1.105955	-0.022266	0.318284
43	1	0	1.469662	0.918250	0.335146
44	6	0	-4.545098	-0.122975	-0.312723
45	6	0	-5.114405	-1.013951	-1.238910
46	6	0	-5.404523	0.745144	0.382518
47	6	0	-6.490869	-1.039374	-1.458472
48	1	0	-4.467275	-1.673700	-1.810513
49	6	0	-6.780711	0.723055	0.160555
50	1	0	-4.991759	1.425265	1.122617
51	6	0	-7.331223	-0.170224	-0.760314
52	1	0	-6.906249	-1.732819	-2.185231
53	1	0	-7.425329	1.399221	0.716293
54	1	0	-8.403968	-0.188311	-0.932650
55	6	0	-0.512306	3.516873	-0.368698
56	1	0	-1.084457	3.336469	-1.274713
57	6	0	3.856888	2.838992	-1.637505
58	1	0	4.683813	3.304211	-1.090432
59	1	0	4.235572	2.510799	-2.611799
60	1	0	3.104681	3.615848	-1.810626

Compound 1b TS180

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1314.75617072 A.U. after 1 cycles
Lowest frequency = -42.0218

Zero-point correction= 0.494005
(Hartree/Particle)
Thermal correction to Energy= 0.519998
Thermal correction to Enthalpy= 0.520942
Thermal correction to Gibbs Free Energy= 0.437115
Sum of electronic and zero-point Energies= -1314.262166
Sum of electronic and thermal Energies= -1314.236173
Sum of electronic and thermal Enthalpies= -1314.235229
Sum of electronic and thermal Free Energies= -1314.319056

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.900627	-4.266116	1.271247
2	6	0	0.548986	-4.557445	1.074275
3	6	0	-0.312644	-3.546188	0.683537
4	6	0	0.143200	-2.232275	0.438864
5	6	0	1.545143	-1.942868	0.527096
6	6	0	-0.840391	-1.162110	0.209306
7	5	0	2.027428	-0.474954	0.210882
8	6	0	-0.413587	0.180809	0.322308
9	6	0	-1.359358	1.241408	0.300124
10	6	0	-0.947232	2.664528	0.468385
11	6	0	-0.231187	3.089206	1.602405

12	6	0	0.120542	4.429659	1.766355
13	6	0	-0.239515	5.373301	0.803030
14	6	0	-0.953540	4.967121	-0.326073
15	6	0	-2.203441	-1.404601	-0.033077
16	6	0	-3.145254	-0.379025	-0.119205
17	6	0	-2.699092	0.940649	0.072705
18	6	0	3.398483	0.210310	-0.314715
19	6	0	4.718211	-0.327655	-0.465326
20	6	0	5.763406	0.495174	-0.911414
21	6	0	5.578687	1.829647	-1.259264
22	6	0	4.297046	2.359091	-1.197209
23	6	0	3.254961	1.554817	-0.746624
24	1	0	2.581785	-5.027607	1.641911
25	1	0	0.162618	-5.555003	1.267107
26	1	0	-1.371087	-3.771092	0.619883
27	1	0	0.030225	2.365286	2.370037
28	1	0	0.668106	4.736804	2.653423
29	1	0	0.033397	6.417207	0.931383
30	1	0	-1.235810	5.694195	-1.083015
31	1	0	-2.551506	-2.424538	-0.145875
32	1	0	-3.412054	1.758514	0.024855
33	1	0	6.759073	0.076903	-1.003409
34	1	0	6.419639	2.428721	-1.599341
35	1	0	4.096337	3.381907	-1.504880
36	1	0	2.273622	2.012464	-0.784087
37	7	0	0.944127	0.451608	0.367822
38	1	0	1.135604	1.444051	0.382791
39	6	0	-4.575892	-0.670303	-0.389980
40	6	0	-4.949276	-1.679115	-1.294827
41	6	0	-5.596856	0.054127	0.249172
42	6	0	-6.291928	-1.956192	-1.547808
43	1	0	-4.177962	-2.232364	-1.823768
44	6	0	-6.939755	-0.219645	-0.006420
45	1	0	-5.334417	0.821252	0.972574
46	6	0	-7.294375	-1.227135	-0.905424
47	1	0	-6.554993	-2.736634	-2.257258
48	1	0	-7.710958	0.349598	0.506229
49	1	0	-8.341046	-1.441416	-1.103887
50	6	0	-1.301203	3.626805	-0.492716
51	1	0	-1.844694	3.312630	-1.379581
52	6	0	5.060787	-1.785323	-0.194820
53	1	0	5.074189	-1.955916	0.890613
54	1	0	4.254053	-2.405860	-0.592870
55	6	0	2.368996	-2.988047	1.000261
56	1	0	3.407125	-2.787401	1.205860
57	6	0	6.383665	-2.314427	-0.765528
58	1	0	6.456825	-2.141553	-1.845080
59	1	0	7.259823	-1.860868	-0.289597
60	1	0	6.446794	-3.394863	-0.595032

Compound 1c GS1

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1582.95652695 A.U. after 1 cycles
Lowest frequency = 7.7344

Zero-point correction= 0.571954
(Hartree/Particle)

Thermal correction to Energy= 0.604473
Thermal correction to Enthalpy= 0.605417
Thermal correction to Gibbs Free Energy= 0.504263
Sum of electronic and zero-point Energies= -1582.384573
Sum of electronic and thermal Energies= -1582.352054
Sum of electronic and thermal Enthalpies= -1582.351110
Sum of electronic and thermal Free Energies= -1582.452264

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.701523	-3.136640	0.345757
2	6	0	1.233611	-4.426056	0.547842
3	6	0	-0.149577	-4.651164	0.574308
4	6	0	-1.039134	-3.600689	0.402671
5	6	0	-0.581560	-2.280108	0.197707
6	6	0	0.822766	-2.048160	0.168023
7	6	0	-1.516715	-1.152579	0.023528
8	6	0	-1.019415	0.166039	-0.159011
9	6	0	-1.916599	1.259352	-0.295950
10	6	0	-1.433952	2.661259	-0.465798
11	6	0	-0.576511	3.263428	0.472914
12	6	0	-0.167115	4.588763	0.319785
13	6	0	-0.609172	5.340470	-0.769877
14	6	0	-1.464065	4.757038	-1.706794
15	6	0	-2.912234	-1.330694	0.034385
16	6	0	-3.812078	-0.278491	-0.126824
17	6	0	-3.286526	1.015178	-0.288425
18	1	0	2.771560	-2.947913	0.319294
19	1	0	1.926407	-5.252478	0.682679
20	1	0	-0.534250	-5.655988	0.731167
21	1	0	-2.100747	-3.819935	0.431450
22	1	0	-0.243225	2.693287	1.336487
23	1	0	0.491908	5.035971	1.059323
24	1	0	-0.289953	6.372367	-0.888224
25	1	0	-1.811105	5.332723	-2.560865
26	1	0	-3.318709	-2.321260	0.199198
27	1	0	-3.962819	1.855601	-0.413968
28	7	0	0.352276	0.375355	-0.225304
29	1	0	0.623003	1.338223	-0.388503
30	6	0	-5.278684	-0.512121	-0.115855
31	6	0	-5.833704	-1.654037	-0.718928
32	6	0	-6.153333	0.401937	0.496585
33	6	0	-7.209925	-1.876320	-0.706165
34	1	0	-5.180476	-2.359666	-1.225002
35	6	0	-7.530096	0.182563	0.506122
36	1	0	-5.746729	1.279473	0.991812
37	6	0	-8.065519	-0.958491	-0.094139
38	1	0	-7.615350	-2.763665	-1.185625
39	1	0	-8.185100	0.900745	0.992746
40	1	0	-9.138505	-1.130195	-0.085909
41	6	0	-1.869905	3.431267	-1.557071
42	1	0	-2.523952	2.976881	-2.296261
43	5	0	1.349210	-0.616364	-0.062524
44	6	0	2.872487	-0.197370	-0.146831
45	6	0	3.669269	-0.408982	-1.315863
46	6	0	3.469241	0.395666	0.960794

47	6	0	3.133845	-1.003289	-2.495979
48	6	0	5.051659	-0.021713	-1.332247
49	6	0	4.835346	0.780066	0.955634
50	6	0	3.912537	-1.202604	-3.613433
51	1	0	2.090277	-1.305987	-2.504320
52	6	0	5.828609	-0.239918	-2.501658
53	6	0	5.600413	0.571362	-0.168563
54	1	0	5.283261	1.241437	1.828513
55	6	0	5.275645	-0.817237	-3.621152
56	1	0	3.478995	-1.659308	-4.499409
57	1	0	6.874167	0.061023	-2.494920
58	1	0	6.647211	0.866931	-0.172018
59	1	0	5.878721	-0.978585	-4.510560
60	8	0	2.636886	0.616619	2.035132
61	6	0	3.162464	0.828587	3.357987
62	1	0	3.911344	1.631987	3.325453
63	6	0	1.977293	1.302685	4.191889
64	1	0	2.292663	1.510139	5.220020
65	1	0	1.549609	2.217104	3.768564
66	1	0	1.196589	0.534985	4.214586
67	6	0	3.793007	-0.450762	3.908306
68	1	0	4.621966	-0.791635	3.280554
69	1	0	4.178628	-0.281137	4.920034
70	1	0	3.044152	-1.249148	3.950346

Compound 1c GS2

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1582.95651684 A.U. after 1 cycles
Lowest frequency = 9.2402

Zero-point correction= 0.572041
(Hartree/Particle)
Thermal correction to Energy= 0.604539
Thermal correction to Enthalpy= 0.605483
Thermal correction to Gibbs Free Energy= 0.504686
Sum of electronic and zero-point Energies= -1582.384476
Sum of electronic and thermal Energies= -1582.351978
Sum of electronic and thermal Enthalpies= -1582.351034
Sum of electronic and thermal Free Energies= -1582.451831

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.585922	-3.015423	-1.197572
2	6	0	1.070935	-4.230901	-1.621500
3	6	0	-0.319676	-4.396836	-1.681107
4	6	0	-1.169594	-3.361194	-1.321818
5	6	0	-0.662888	-2.116478	-0.886510
6	6	0	0.748196	-1.945087	-0.824265
7	6	0	-1.556280	-1.005634	-0.504994
8	5	0	1.328082	-0.594993	-0.353604
9	6	0	-1.012165	0.248575	-0.118276
10	6	0	-1.868880	1.327823	0.226748
11	6	0	-1.335236	2.662441	0.629645
12	6	0	-1.701057	3.225406	1.863781

13	6	0	-1.244973	4.488931	2.238528
14	6	0	-0.408748	5.215074	1.388423
15	6	0	-0.036733	4.670137	0.158613
16	6	0	-2.956784	-1.138057	-0.509079
17	6	0	-3.817665	-0.101942	-0.150444
18	6	0	-3.246222	1.129325	0.214183
19	1	0	2.662041	-2.870388	-1.150584
20	1	0	1.732746	-5.044207	-1.907564
21	1	0	-0.741074	-5.342027	-2.014723
22	1	0	-2.238628	-3.530467	-1.388701
23	1	0	-2.340603	2.657660	2.534103
24	1	0	-1.538536	4.903763	3.199302
25	1	0	-0.050288	6.197997	1.681827
26	1	0	0.606886	5.230027	-0.514604
27	1	0	-3.399144	-2.075965	-0.822469
28	1	0	-3.890875	1.954833	0.501281
29	7	0	0.368413	0.403985	-0.054718
30	1	0	0.672761	1.313770	0.273098
31	6	0	-5.291148	-0.287532	-0.161095
32	6	0	-6.147588	0.742202	-0.587371
33	6	0	-5.870992	-1.498123	0.255969
34	6	0	-7.530816	0.568161	-0.596813
35	1	0	-5.722480	1.678431	-0.938650
36	6	0	-7.253848	-1.674461	0.242910
37	1	0	-5.231058	-2.298090	0.618293
38	6	0	-8.091143	-0.641660	-0.182888
39	1	0	-8.171673	1.377138	-0.938079
40	1	0	-7.678410	-2.617801	0.576822
41	1	0	-9.169201	-0.777939	-0.191277
42	6	0	-0.497304	3.407981	-0.218894
43	1	0	-0.222039	3.004232	-1.189823
44	6	0	2.863906	-0.240458	-0.224282
45	6	0	3.549803	0.573689	-1.178661
46	6	0	3.581415	-0.735297	0.861586
47	6	0	2.894488	1.111728	-2.326020
48	6	0	4.946214	0.866279	-1.012866
49	6	0	4.961335	-0.452312	1.033915
50	6	0	3.569845	1.890955	-3.237698
51	1	0	1.841034	0.893820	-2.478656
52	6	0	5.614213	1.675834	-1.970920
53	6	0	5.618560	0.330467	0.112080
54	1	0	5.505285	-0.838468	1.887901
55	6	0	4.945300	2.181343	-3.061165
56	1	0	3.045398	2.285432	-4.104374
57	1	0	6.671586	1.887156	-1.825486
58	1	0	6.675483	0.549243	0.246913
59	1	0	5.466452	2.797879	-3.788490
60	8	0	2.852481	-1.499516	1.737262
61	6	0	3.458664	-2.144700	2.870642
62	1	0	4.449509	-2.519319	2.580558
63	6	0	2.559026	-3.332793	3.196179
64	1	0	2.963452	-3.897850	4.043075
65	1	0	1.552872	-2.987416	3.456812
66	1	0	2.478065	-4.000027	2.333051
67	6	0	3.584885	-1.167463	4.040456
68	1	0	4.041720	-1.662086	4.905357
69	1	0	4.198750	-0.300259	3.778708
70	1	0	2.593010	-0.805875	4.332818

Compound 1c GS3

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1582.95499608 A.U. after 1 cycles
Lowest frequency = 13.2401

Zero-point correction= 0.571938
(Hartree/Particle)
Thermal correction to Energy= 0.604367
Thermal correction to Enthalpy= 0.605312
Thermal correction to Gibbs Free Energy= 0.505439
Sum of electronic and zero-point Energies= -1582.383058
Sum of electronic and thermal Energies= -1582.350629
Sum of electronic and thermal Enthalpies= -1582.349685
Sum of electronic and thermal Free Energies= -1582.449557

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.769035	-3.100767	0.387269
2	6	0	1.308192	-4.393558	0.582622
3	6	0	-0.073279	-4.630950	0.576816
4	6	0	-0.967624	-3.588790	0.382574
5	6	0	-0.518464	-2.263942	0.185067
6	6	0	0.885148	-2.019480	0.183274
7	6	0	-1.462002	-1.145975	-0.003538
8	6	0	-0.975147	0.179356	-0.164294
9	6	0	-1.879268	1.266372	-0.311293
10	6	0	-1.409484	2.673793	-0.472919
11	6	0	-0.547129	3.280600	0.458636
12	6	0	-0.152439	4.610571	0.305576
13	6	0	-0.614547	5.362808	-0.775046
14	6	0	-1.474187	4.774814	-1.704852
15	6	0	-2.855612	-1.339050	-0.022228
16	6	0	-3.761889	-0.293820	-0.190309
17	6	0	-3.246262	1.006589	-0.330338
18	1	0	2.838097	-2.904660	0.384597
19	1	0	2.005190	-5.212814	0.737254
20	1	0	-0.452637	-5.638609	0.727708
21	1	0	-2.027559	-3.817104	0.390118
22	1	0	-0.191900	2.714710	1.315894
23	1	0	0.512459	5.058926	1.038882
24	1	0	-0.306506	6.398174	-0.892715
25	1	0	-1.836271	5.350125	-2.552917
26	1	0	-3.255684	-2.334999	0.124476
27	1	0	-3.929348	1.840547	-0.461332
28	7	0	0.395105	0.401308	-0.197012
29	1	0	0.662146	1.369195	-0.335650
30	6	0	-5.226189	-0.541306	-0.208896
31	6	0	-5.758973	-1.681403	-0.834896
32	6	0	-6.120206	0.357560	0.397913
33	6	0	-7.133008	-1.916705	-0.849641
34	1	0	-5.090014	-2.374841	-1.337287
35	6	0	-7.494715	0.124998	0.380160
36	1	0	-5.731068	1.233236	0.910162
37	6	0	-8.008130	-1.014076	-0.242661

38	1	0	-7.521271	-2.802096	-1.346548
39	1	0	-8.165265	0.831277	0.862938
40	1	0	-9.079373	-1.195933	-0.255818
41	6	0	-1.864741	3.444623	-1.556286
42	1	0	-2.520941	2.986892	-2.291479
43	5	0	1.400475	-0.580295	-0.031180
44	6	0	2.910011	-0.106792	-0.064746
45	6	0	3.798454	-0.439610	-1.144837
46	6	0	3.399585	0.712294	0.945235
47	6	0	3.384362	-1.254418	-2.237600
48	6	0	5.140280	0.071041	-1.164889
49	6	0	4.719995	1.228062	0.926090
50	6	0	4.241392	-1.558300	-3.272103
51	1	0	2.371526	-1.646175	-2.246672
52	6	0	6.000366	-0.261089	-2.245693
53	6	0	5.569524	0.913121	-0.105932
54	1	0	5.030096	1.880747	1.736242
55	6	0	5.565701	-1.059661	-3.278459
56	1	0	3.898689	-2.185088	-4.091228
57	1	0	7.014105	0.133620	-2.242461
58	1	0	6.582198	1.309475	-0.125423
59	1	0	6.233291	-1.305805	-4.099817
60	8	0	2.581906	1.114015	1.990723
61	6	0	2.386256	0.170482	3.074141
62	1	0	2.177627	-0.815783	2.637566
63	6	0	3.631526	0.078846	3.955157
64	1	0	3.471272	-0.643231	4.764167
65	1	0	4.502597	-0.248181	3.378596
66	1	0	3.857653	1.054033	4.401838
67	6	0	1.160997	0.655501	3.837996
68	1	0	0.283135	0.679006	3.185085
69	1	0	0.947400	-0.009837	4.681502
70	1	0	1.331839	1.664956	4.229110

Compound 1c TS0

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1582.91794657 A.U. after 1 cycles
Lowest frequency = -44.8467

Zero-point correction= 0.571985
(Hartree/Particle)
Thermal correction to Energy= 0.603498
Thermal correction to Enthalpy= 0.604442
Thermal correction to Gibbs Free Energy= 0.507525
Sum of electronic and zero-point Energies= -1582.345961
Sum of electronic and thermal Energies= -1582.314449
Sum of electronic and thermal Enthalpies= -1582.313505
Sum of electronic and thermal Free Energies= -1582.410422

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.691275	-3.501461	-0.702771
2	6	0	-1.149361	-4.777267	-0.756083
3	6	0	0.208887	-4.956707	-0.486355

4	6	0	1.002672	-3.845717	-0.261901
5	6	0	0.472430	-2.535721	-0.246700
6	6	0	-0.945026	-2.344818	-0.380498
7	6	0	1.399543	-1.392388	-0.216923
8	6	0	0.890145	-0.103328	-0.496941
9	6	0	1.772845	0.996080	-0.688523
10	6	0	1.285954	2.349180	-1.081154
11	6	0	0.426903	2.527109	-2.180433
12	6	0	0.018254	3.802355	-2.570774
13	6	0	0.461822	4.927824	-1.874504
14	6	0	1.318697	4.767649	-0.783989
15	6	0	2.784329	-1.525737	-0.012988
16	6	0	3.666460	-0.451410	-0.126019
17	6	0	3.136865	0.798684	-0.490910
18	1	0	-2.725827	-3.401724	-0.986822
19	1	0	-1.778802	-5.623616	-1.017968
20	1	0	0.653375	-5.948501	-0.501839
21	1	0	2.069375	-3.997533	-0.147055
22	1	0	0.093335	1.659581	-2.742943
23	1	0	-0.641214	3.915540	-3.427224
24	1	0	0.143501	5.921021	-2.179630
25	1	0	1.669198	5.636900	-0.233439
26	1	0	3.200830	-2.497688	0.221870
27	1	0	3.805854	1.644848	-0.615915
28	7	0	-0.480355	0.086515	-0.500158
29	1	0	-0.724162	1.067682	-0.456377
30	6	0	5.122602	-0.626477	0.106919
31	6	0	5.594407	-1.467919	1.129343
32	6	0	6.070329	0.043513	-0.686024
33	6	0	6.960869	-1.636628	1.348143
34	1	0	4.880872	-1.973610	1.774331
35	6	0	7.436957	-0.121477	-0.465229
36	1	0	5.731810	0.678907	-1.499832
37	6	0	7.889555	-0.963340	0.552362
38	1	0	7.300308	-2.287719	2.149727
39	1	0	8.150032	0.401801	-1.097156
40	1	0	8.954772	-1.092952	0.723716
41	6	0	1.724466	3.492600	-0.391605
42	1	0	2.381194	3.374260	0.465937
43	5	0	-1.502221	-0.872263	-0.225424
44	6	0	-2.908230	-0.164267	0.193855
45	6	0	-4.268907	-0.617403	-0.076603
46	6	0	-2.845660	1.126948	0.749988
47	6	0	-4.614566	-1.984135	-0.245340
48	6	0	-5.376938	0.301956	-0.092555
49	6	0	-3.948431	2.020941	0.790610
50	6	0	-5.894741	-2.402436	-0.544074
51	1	0	-3.866532	-2.728184	-0.039568
52	6	0	-6.678508	-0.140618	-0.447674
53	6	0	-5.172094	1.642943	0.315390
54	1	0	-3.772505	3.028522	1.154687
55	6	0	-6.939940	-1.467874	-0.695338
56	1	0	-6.100531	-3.465522	-0.639602
57	1	0	-7.477385	0.596730	-0.485270
58	1	0	-6.002464	2.344327	0.285321
59	1	0	-7.942097	-1.797730	-0.954468
60	8	0	-1.659184	1.662409	1.226205
61	6	0	-1.574695	1.886853	2.656182
62	1	0	-2.518437	2.342437	2.988169

63	6	0	-1.364787	0.567201	3.395391
64	1	0	-1.331819	0.740103	4.477386
65	1	0	-2.178744	-0.134201	3.187162
66	1	0	-0.421462	0.102128	3.088917
67	6	0	-0.433645	2.874025	2.861625
68	1	0	-0.614199	3.796872	2.302123
69	1	0	-0.330577	3.119542	3.924211
70	1	0	0.510245	2.441801	2.512731

Compound 1c TS180

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1582.92232010 A.U. after 1 cycles
Lowest frequency = -19.1445

Zero-point correction= 0.572512
(Hartree/Particle)
Thermal correction to Energy= 0.603728
Thermal correction to Enthalpy= 0.604672
Thermal correction to Gibbs Free Energy= 0.509886
Sum of electronic and zero-point Energies= -1582.349808
Sum of electronic and thermal Energies= -1582.318592
Sum of electronic and thermal Enthalpies= -1582.317648
Sum of electronic and thermal Free Energies= -1582.412434

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.759900	-3.016354	0.979779
2	6	0	-1.316690	-4.290454	1.304704
3	6	0	0.035752	-4.610851	1.151624
4	6	0	0.923855	-3.629185	0.746627
5	6	0	0.492479	-2.316671	0.450880
6	6	0	-0.901912	-2.003240	0.497824
7	6	0	1.496196	-1.265282	0.224309
8	6	0	1.093701	0.086847	0.332107
9	6	0	2.067471	1.123131	0.329600
10	6	0	1.704369	2.551718	0.553694
11	6	0	2.092915	3.538556	-0.368146
12	6	0	1.801233	4.884119	-0.143114
13	6	0	1.110057	5.269994	1.007348
14	6	0	0.716977	4.301093	1.932123
15	6	0	2.853500	-1.538344	-0.015556
16	6	0	3.819485	-0.534993	-0.095338
17	6	0	3.401504	0.792516	0.106151
18	1	0	-2.805014	-2.788431	1.114742
19	1	0	-2.016901	-5.031022	1.683952
20	1	0	0.399464	-5.607757	1.388211
21	1	0	1.980611	-3.870071	0.716237
22	1	0	2.621947	3.240494	-1.269387
23	1	0	2.112658	5.631314	-0.868654
24	1	0	0.881730	6.317806	1.182802
25	1	0	0.185636	4.592116	2.834272
26	1	0	3.164260	-2.562943	-0.184617
27	1	0	4.140812	1.587849	0.125029
28	7	0	-0.260326	0.385570	0.357338

29	1	0	-0.445259	1.378912	0.402290
30	6	0	5.244209	-0.854503	-0.363338
31	6	0	5.843889	-2.008364	0.170740
32	6	0	6.036167	-0.009793	-1.160530
33	6	0	7.180588	-2.308896	-0.086528
34	1	0	5.262051	-2.661206	0.815533
35	6	0	7.374321	-0.306727	-1.414517
36	1	0	5.589422	0.875332	-1.605109
37	6	0	7.953434	-1.459068	-0.880003
38	1	0	7.622391	-3.203976	0.343976
39	1	0	7.963183	0.359339	-2.040062
40	1	0	8.996155	-1.691745	-1.078664
41	6	0	1.012774	2.956363	1.709215
42	1	0	0.723707	2.210851	2.445462
43	5	0	-1.351564	-0.527573	0.167747
44	6	0	-2.769334	0.114769	-0.209502
45	6	0	-2.942181	1.553074	-0.401830
46	6	0	-3.970455	-0.620321	-0.284658
47	6	0	-1.913116	2.420233	-0.880696
48	6	0	-4.226246	2.175861	-0.219257
49	6	0	-5.247529	-0.009275	-0.135636
50	6	0	-2.090018	3.784199	-1.004603
51	1	0	-0.987970	1.997227	-1.249918
52	6	0	-4.373979	3.584245	-0.311291
53	6	0	-5.359508	1.350541	-0.027209
54	1	0	-6.136568	-0.622633	-0.065792
55	6	0	-3.318604	4.390118	-0.670189
56	1	0	-1.272002	4.389677	-1.384608
57	1	0	-5.358291	4.009873	-0.127852
58	1	0	-6.330693	1.809263	0.143036
59	1	0	-3.442318	5.466445	-0.749491
60	8	0	-3.880092	-1.961458	-0.497150
61	6	0	-5.021927	-2.766104	-0.859958
62	1	0	-5.725329	-2.142961	-1.425760
63	6	0	-4.477430	-3.856986	-1.777842
64	1	0	-5.287355	-4.520187	-2.101296
65	1	0	-4.011654	-3.415518	-2.663769
66	1	0	-3.722513	-4.453399	-1.255551
67	6	0	-5.706404	-3.337534	0.383382
68	1	0	-6.027102	-2.549647	1.071825
69	1	0	-6.589475	-3.919324	0.095284
70	1	0	-5.022606	-4.001734	0.922781

Compound 1d GS1

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1429.11402926 A.U. after 1 cycles
Lowest frequency = 10.9465

Zero-point correction= 0.510582
(Hartree/Particle)
Thermal correction to Energy= 0.539449
Thermal correction to Enthalpy= 0.540393
Thermal correction to Gibbs Free Energy= 0.447836
Sum of electronic and zero-point Energies= -1428.603448
Sum of electronic and thermal Energies= -1428.574580
Sum of electronic and thermal Enthalpies= -1428.573636
Sum of electronic and thermal Free Energies= -1428.666193

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.804211	-3.363376	-0.361865
2	6	0	-1.262977	-4.638096	-0.294952
3	6	0	0.126344	-4.781609	-0.178482
4	6	0	0.949887	-3.666356	-0.128120
5	6	0	0.417560	-2.359964	-0.195773
6	6	0	-0.993149	-2.210257	-0.318109
7	6	0	1.281329	-1.165436	-0.138755
8	6	0	0.711588	0.132978	-0.224182
9	6	0	1.540605	1.285430	-0.186720
10	6	0	0.977956	2.664624	-0.286467
11	6	0	0.235452	3.074559	-1.408174
12	6	0	-0.253569	4.378048	-1.504693
13	6	0	-0.006300	5.298207	-0.484820
14	6	0	0.734506	4.906582	0.631827
15	6	0	2.678142	-1.259210	0.002849
16	6	0	3.510040	-0.142833	0.067938
17	6	0	2.913941	1.126567	-0.030388
18	1	0	-2.880123	-3.236148	-0.449766
19	1	0	-1.903912	-5.514942	-0.330304
20	1	0	0.567957	-5.773692	-0.125249
21	1	0	2.018880	-3.823902	-0.037507
22	1	0	0.061510	2.371985	-2.219325
23	1	0	-0.820373	4.675933	-2.382792
24	1	0	-0.387296	6.312989	-0.560039
25	1	0	0.930394	5.615645	1.431844
26	1	0	3.142320	-2.237215	0.042277
27	1	0	3.535546	2.015673	0.019907
28	7	0	-0.669941	0.269058	-0.321780
29	1	0	-0.994474	1.229664	-0.339632
30	6	0	4.979767	-0.286847	0.226104
31	6	0	5.523795	-1.281428	1.056950
32	6	0	5.867519	0.567825	-0.449752
33	6	0	6.903329	-1.419591	1.203048
34	1	0	4.856820	-1.934402	1.613293
35	6	0	7.247140	0.432753	-0.301184
36	1	0	5.471933	1.328274	-1.117495
37	6	0	7.772146	-0.562528	0.525090
38	1	0	7.299741	-2.192078	1.857013
39	1	0	7.913499	1.101142	-0.840390
40	1	0	8.847449	-0.668581	0.640282
41	6	0	1.219856	3.602768	0.730538
42	1	0	1.785367	3.297983	1.606882
43	5	0	-1.604489	-0.794408	-0.381888
44	6	0	-3.146619	-0.456203	-0.497850
45	6	0	-3.898284	-0.105312	0.677190
46	6	0	-3.794980	-0.481359	-1.730801
47	6	0	-3.303530	-0.069691	1.971075
48	6	0	-5.292062	0.215915	0.575488
49	6	0	-5.178218	-0.161273	-1.816166
50	6	0	-4.034597	0.264606	3.089604
51	1	0	-2.249020	-0.311597	2.073130
52	6	0	-6.020512	0.557240	1.746227
53	6	0	-5.906185	0.178109	-0.703000

54	1	0	-5.662563	-0.188978	-2.790159
55	6	0	-5.408918	0.583253	2.978778
56	1	0	-3.554824	0.283023	4.064691
57	1	0	-7.077011	0.798194	1.649334
58	1	0	-6.964065	0.417672	-0.786722
59	1	0	-5.976934	0.845940	3.867278
60	6	0	-3.060122	-0.804001	-3.015880
61	1	0	-2.708421	0.110741	-3.513275
62	1	0	-2.185292	-1.438128	-2.844440
63	1	0	-3.715095	-1.321122	-3.726366

Compound 1d GS2

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1429.11424051 A.U. after 1 cycles
Lowest frequency = 10.1530

Zero-point correction= 0.510608
(Hartree/Particle)
Thermal correction to Energy= 0.539468
Thermal correction to Enthalpy= 0.540412
Thermal correction to Gibbs Free Energy= 0.447853
Sum of electronic and zero-point Energies= -1428.603632
Sum of electronic and thermal Energies= -1428.574772
Sum of electronic and thermal Enthalpies= -1428.573828
Sum of electronic and thermal Free Energies= -1428.666387

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.776188	-3.392752	-0.114914
2	6	0	-1.230751	-4.654184	0.068541
3	6	0	0.156017	-4.778473	0.229403
4	6	0	0.973310	-3.657702	0.205872
5	6	0	0.436709	-2.364653	0.019703
6	6	0	-0.971740	-2.234572	-0.144457
7	6	0	1.293429	-1.163788	-0.001783
8	6	0	0.713831	0.124866	-0.148067
9	6	0	1.531763	1.286025	-0.143760
10	6	0	0.957278	2.656733	-0.283356
11	6	0	1.398923	3.506023	-1.311603
12	6	0	0.901836	4.803496	-1.431927
13	6	0	-0.051249	5.277688	-0.528584
14	6	0	-0.499347	4.446596	0.499195
15	6	0	2.692915	-1.241997	0.120882
16	6	0	3.519083	-0.119622	0.101690
17	6	0	2.911016	1.140919	-0.030603
18	1	0	-2.850176	-3.280192	-0.239241
19	1	0	-1.866530	-5.535219	0.090121
20	1	0	0.600445	-5.759707	0.376883
21	1	0	2.040047	-3.799880	0.338708
22	1	0	2.130679	3.136081	-2.024609
23	1	0	1.255370	5.442596	-2.236799
24	1	0	-0.441224	6.287324	-0.624475
25	1	0	-1.234304	4.808552	1.213135
26	1	0	3.159610	-2.209912	0.258172

27	1	0	3.528793	2.033859	-0.050701
28	7	0	-0.661924	0.239755	-0.322060
29	1	0	-0.987975	1.190587	-0.455702
30	6	0	4.993491	-0.247625	0.226710
31	6	0	5.740551	0.683914	0.967980
32	6	0	5.682927	-1.303677	-0.393689
33	6	0	7.124565	0.563720	1.085234
34	1	0	5.227563	1.494745	1.477919
35	6	0	7.066399	-1.426750	-0.273688
36	1	0	5.130584	-2.018831	-0.997190
37	6	0	7.794456	-0.493028	0.465976
38	1	0	7.679404	1.292623	1.670363
39	1	0	7.577738	-2.248356	-0.768714
40	1	0	8.873064	-0.587438	0.558096
41	6	0	0.001526	3.149863	0.622983
42	1	0	-0.335138	2.519753	1.442284
43	5	0	-1.586214	-0.833767	-0.347491
44	6	0	-3.121135	-0.514998	-0.566932
45	6	0	-3.933193	-0.093485	0.542497
46	6	0	-3.702796	-0.617500	-1.828729
47	6	0	-3.408565	0.019584	1.862279
48	6	0	-5.318221	0.222113	0.346974
49	6	0	-5.078485	-0.303844	-2.007107
50	6	0	-4.196560	0.423178	2.917578
51	1	0	-2.363474	-0.222954	2.036091
52	6	0	-6.106229	0.636438	1.453985
53	6	0	-5.863400	0.105162	-0.957635
54	1	0	-5.510544	-0.392211	-3.001794
55	6	0	-5.561276	0.737694	2.713628
56	1	0	-3.770335	0.497955	3.914676
57	1	0	-7.154986	0.872195	1.286159
58	1	0	-6.914298	0.339834	-1.112635
59	1	0	-6.174755	1.055214	3.552614
60	6	0	-2.898899	-1.019700	-3.048219
61	1	0	-2.486089	-0.139706	-3.560639
62	1	0	-2.057411	-1.670206	-2.791326
63	1	0	-3.523470	-1.550134	-3.775851

Compound 1d GS3

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1429.11416381 A.U. after 1 cycles
Lowest frequency = 10.8149

Zero-point correction= 0.510586
(Hartree/Particle)
Thermal correction to Energy= 0.539447
Thermal correction to Enthalpy= 0.540391
Thermal correction to Gibbs Free Energy= 0.447890
Sum of electronic and zero-point Energies= -1428.603578
Sum of electronic and thermal Energies= -1428.574717
Sum of electronic and thermal Enthalpies= -1428.573773
Sum of electronic and thermal Free Energies= -1428.666274

Standard orientation:

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

1	6	0	-1.779487	-3.382372	-0.278162
2	6	0	-1.235844	-4.651614	-0.152253
3	6	0	0.150112	-4.784804	0.008551
4	6	0	0.968422	-3.665012	0.040930
5	6	0	0.433871	-2.364193	-0.088157
6	6	0	-0.973863	-2.224964	-0.250846
7	6	0	1.291703	-1.164672	-0.048398
8	6	0	0.714629	0.129879	-0.141800
9	6	0	1.534817	1.288358	-0.091026
10	6	0	0.960289	2.664713	-0.152066
11	6	0	1.396274	3.567894	-1.135780
12	6	0	0.899773	4.870277	-1.183383
13	6	0	-0.047266	5.295721	-0.249970
14	6	0	-0.489927	4.410756	0.734320
15	6	0	2.691279	-1.250489	0.068892
16	6	0	3.519504	-0.129910	0.097113
17	6	0	2.913926	1.136497	0.015607
18	1	0	-2.852934	-3.262930	-0.400673
19	1	0	-1.872482	-5.532010	-0.174522
20	1	0	0.593033	-5.772341	0.111862
21	1	0	2.034266	-3.814055	0.173462
22	1	0	2.123204	3.236115	-1.872179
23	1	0	1.248919	5.551562	-1.954887
24	1	0	-0.436814	6.309308	-0.288955
25	1	0	-1.220127	4.734313	1.471191
26	1	0	3.160466	-2.226169	0.106955
27	1	0	3.529106	2.028820	0.083444
28	7	0	-0.660815	0.254577	-0.311466
29	1	0	-0.984965	1.210903	-0.404155
30	6	0	4.993426	-0.265283	0.218201
31	6	0	5.566142	-1.254378	1.036180
32	6	0	5.857427	0.593407	-0.482853
33	6	0	6.949963	-1.383741	1.144880
34	1	0	4.918913	-1.909808	1.612515
35	6	0	7.241341	0.467412	-0.371723
36	1	0	5.438820	1.350539	-1.140298
37	6	0	7.794777	-0.522960	0.441805
38	1	0	7.368762	-2.152144	1.789626
39	1	0	7.888647	1.139049	-0.929781
40	1	0	8.873437	-0.622081	0.528046
41	6	0	0.010335	3.108977	0.785103
42	1	0	-0.322159	2.435740	1.571064
43	5	0	-1.586382	-0.815401	-0.389190
44	6	0	-3.120351	-0.485034	-0.597794
45	6	0	-3.934316	-0.110700	0.527115
46	6	0	-3.699448	-0.532158	-1.864070
47	6	0	-3.412458	-0.055075	1.851648
48	6	0	-5.318623	0.214522	0.342488
49	6	0	-5.074460	-0.209555	-2.031576
50	6	0	-4.202301	0.303669	2.921675
51	1	0	-2.367962	-0.305859	2.017069
52	6	0	-6.108611	0.581631	1.464632
53	6	0	-5.861188	0.154519	-0.967063
54	1	0	-5.504479	-0.254359	-3.030057
55	6	0	-5.566270	0.628081	2.728605
56	1	0	-3.778101	0.335169	3.921939
57	1	0	-7.156775	0.825494	1.304883
58	1	0	-6.911532	0.396777	-1.113925

59	1	0	-6.181224	0.909919	3.579175
60	6	0	-2.893660	-0.881681	-3.098448
61	1	0	-2.483068	0.019871	-3.573859
62	1	0	-2.050563	-1.539943	-2.868164
63	1	0	-3.516378	-1.383247	-3.847826

Compound 1d GS4

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1429.11395868 A.U. after 1 cycles
Lowest frequency = 10.5849

Zero-point correction= 0.510562
(Hartree/Particle)
Thermal correction to Energy= 0.539435
Thermal correction to Enthalpy= 0.540379
Thermal correction to Gibbs Free Energy= 0.447775
Sum of electronic and zero-point Energies= -1428.603396
Sum of electronic and thermal Energies= -1428.574524
Sum of electronic and thermal Enthalpies= -1428.573580
Sum of electronic and thermal Free Energies= -1428.666184

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.801218	-3.376607	-0.196285
2	6	0	-1.258413	-4.646197	-0.070469
3	6	0	0.131541	-4.782879	0.046719
4	6	0	0.954149	-3.665819	0.040409
5	6	0	0.420077	-2.364501	-0.085783
6	6	0	-0.991190	-2.222007	-0.210158
7	6	0	1.282949	-1.168005	-0.090908
8	6	0	0.711126	0.124726	-0.230177
9	6	0	1.538167	1.279167	-0.239729
10	6	0	0.974891	2.650015	-0.418626
11	6	0	0.238365	2.997865	-1.564956
12	6	0	-0.250781	4.293723	-1.734740
13	6	0	-0.009964	5.268102	-0.764849
14	6	0	0.724526	4.938320	0.375635
15	6	0	2.679775	-1.253351	0.056146
16	6	0	3.510113	-0.134122	0.073079
17	6	0	2.911862	1.129550	-0.076849
18	1	0	-2.877554	-3.254682	-0.286492
19	1	0	-1.898570	-5.524275	-0.061417
20	1	0	0.574371	-5.770944	0.145251
21	1	0	2.023832	-3.818027	0.131963
22	1	0	0.069279	2.252049	-2.337557
23	1	0	-0.812577	4.543139	-2.630963
24	1	0	-0.391099	6.276964	-0.897210
25	1	0	0.915216	5.689893	1.137187
26	1	0	3.138985	-2.224560	0.195282
27	1	0	3.537189	2.016594	-0.114749
28	7	0	-0.670659	0.254592	-0.332735
29	1	0	-0.996438	1.213080	-0.392445
30	6	0	4.980127	-0.268945	0.235283
31	6	0	5.710669	0.659145	0.997043

32	6	0	5.682256	-1.326901	-0.367336
33	6	0	7.090437	0.533764	1.151868
34	1	0	5.186984	1.472081	1.492627
35	6	0	7.061446	-1.455409	-0.209799
36	1	0	5.144157	-2.039136	-0.986878
37	6	0	7.772787	-0.525211	0.550259
38	1	0	7.632076	1.260343	1.752067
39	1	0	7.582911	-2.278427	-0.691722
40	1	0	8.848129	-0.623827	0.671447
41	6	0	1.210135	3.642204	0.547321
42	1	0	1.770547	3.385630	1.442231
43	5	0	-1.604148	-0.811471	-0.340201
44	6	0	-3.146927	-0.480863	-0.468390
45	6	0	-3.898106	-0.082893	0.691747
46	6	0	-3.796267	-0.558486	-1.698624
47	6	0	-3.302151	0.007543	1.982414
48	6	0	-5.292557	0.231360	0.578134
49	6	0	-5.180111	-0.244633	-1.795943
50	6	0	-4.032825	0.386547	3.086837
51	1	0	-2.247104	-0.228101	2.093389
52	6	0	-6.020556	0.619630	1.734453
53	6	0	-5.907697	0.139446	-0.697099
54	1	0	-5.665302	-0.313721	-2.767450
55	6	0	-5.407866	0.697793	2.964245
56	1	0	-3.552234	0.446170	4.059870
57	1	0	-7.077584	0.854466	1.628715
58	1	0	-6.966081	0.373446	-0.789695
59	1	0	-5.975558	0.996008	3.841669
60	6	0	-3.061433	-0.933594	-2.969410
61	1	0	-2.704377	-0.040415	-3.500999
62	1	0	-2.189922	-1.564914	-2.772292
63	1	0	-3.717943	-1.474485	-3.660468

Compound 1d TS0

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1429.07321679 A.U. after 1 cycles
Lowest frequency = -27.7994

Zero-point correction= 0.511521
(Hartree/Particle)
Thermal correction to Energy= 0.538844
Thermal correction to Enthalpy= 0.539788
Thermal correction to Gibbs Free Energy= 0.453656
Sum of electronic and zero-point Energies= -1428.561696
Sum of electronic and thermal Energies= -1428.534373
Sum of electronic and thermal Enthalpies= -1428.533428
Sum of electronic and thermal Free Energies= -1428.619561

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.932335	-3.163810	-0.732172
2	6	0	-1.435959	-4.431758	-1.000517
3	6	0	-0.073206	-4.686813	-0.829398
4	6	0	0.772206	-3.646581	-0.481963

5	6	0	0.288365	-2.340582	-0.246809
6	6	0	-1.123953	-2.094859	-0.283644
7	6	0	1.249836	-1.234273	-0.099694
8	6	0	0.777706	0.092884	-0.233496
9	6	0	1.691893	1.176977	-0.325629
10	6	0	1.236021	2.578294	-0.550919
11	6	0	0.400853	2.909970	-1.633234
12	6	0	0.007947	4.230254	-1.856125
13	6	0	0.444875	5.247043	-1.005585
14	6	0	1.279212	4.933996	0.069617
15	6	0	2.631227	-1.429895	0.067490
16	6	0	3.546387	-0.376592	0.051825
17	6	0	3.052046	0.919943	-0.172769
18	1	0	-2.978123	-2.987279	-0.932327
19	1	0	-2.104207	-5.213360	-1.352301
20	1	0	0.333703	-5.677263	-1.016353
21	1	0	1.837883	-3.842111	-0.449828
22	1	0	0.075848	2.128774	-2.315367
23	1	0	-0.633177	4.464053	-2.701897
24	1	0	0.139280	6.275114	-1.179774
25	1	0	1.623405	5.718278	0.738751
26	1	0	3.015809	-2.434567	0.197143
27	1	0	3.744293	1.755653	-0.214636
28	7	0	-0.588834	0.319045	-0.186321
29	1	0	-0.827448	1.302044	-0.182186
30	6	0	4.998690	-0.618372	0.245253
31	6	0	5.454672	-1.573104	1.170637
32	6	0	5.957892	0.099929	-0.489317
33	6	0	6.817524	-1.803827	1.352123
34	1	0	4.732784	-2.119930	1.771206
35	6	0	7.321024	-0.127510	-0.305537
36	1	0	5.630421	0.824391	-1.229968
37	6	0	7.757976	-1.081386	0.615449
38	1	0	7.145228	-2.542615	2.079031
39	1	0	8.043218	0.435479	-0.891249
40	1	0	8.820404	-1.259559	0.757960
41	6	0	1.668749	3.613972	0.295309
42	1	0	2.305528	3.373510	1.142270
43	5	0	-1.623997	-0.639826	0.063730
44	6	0	-2.982133	0.052614	0.587703
45	6	0	-4.335445	-0.422769	0.335115
46	6	0	-2.897328	1.331920	1.178511
47	6	0	-4.672588	-1.800851	0.264094
48	6	0	-5.437456	0.496034	0.269304
49	6	0	-4.016484	2.211546	1.175306
50	6	0	-5.953849	-2.235059	-0.009355
51	1	0	-3.919780	-2.527957	0.526684
52	6	0	-6.736828	0.034086	-0.068938
53	6	0	-5.224129	1.845978	0.644780
54	1	0	-3.886725	3.209525	1.588911
55	6	0	-6.994339	-1.307824	-0.231784
56	1	0	-6.166948	-3.300894	-0.025894
57	1	0	-7.538235	0.764994	-0.152053
58	1	0	-6.049491	2.552220	0.590227
59	1	0	-7.995706	-1.653799	-0.472845
60	6	0	-1.692561	1.872622	1.938838
61	1	0	-0.945119	1.109843	2.156605
62	1	0	-1.191871	2.706802	1.429439
63	1	0	-2.048198	2.271294	2.897246

Compound 1d TS180

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -1429.07394068 A.U. after 1 cycles
Lowest frequency = -33.5667

Zero-point correction= 0.511701
(Hartree/Particle)
Thermal correction to Energy= 0.538904
Thermal correction to Enthalpy= 0.539848
Thermal correction to Gibbs Free Energy= 0.454087
Sum of electronic and zero-point Energies= -1428.562239
Sum of electronic and thermal Energies= -1428.535036
Sum of electronic and thermal Enthalpies= -1428.534092
Sum of electronic and thermal Free Energies= -1428.619854

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.316652	3.949760	0.634200
2	6	0	0.546672	5.092203	0.802514
3	6	0	-0.831836	5.028469	0.584255
4	6	0	-1.415847	3.807507	0.290896
5	6	0	-0.648778	2.629029	0.158414
6	6	0	0.778965	2.704036	0.244717
7	6	0	-1.334701	1.329773	0.075445
8	6	0	-0.586323	0.154405	0.322005
9	6	0	-1.245316	-1.097883	0.464552
10	6	0	-0.513027	-2.343729	0.829221
11	6	0	-0.678129	-3.513391	0.067846
12	6	0	-0.034322	-4.697746	0.424237
13	6	0	0.792939	-4.736800	1.548359
14	6	0	0.965375	-3.584223	2.316179
15	6	0	-2.715959	1.203079	-0.149976
16	6	0	-3.377715	-0.023080	-0.085135
17	6	0	-2.619980	-1.159435	0.249270
18	1	0	2.368102	4.020879	0.858877
19	1	0	1.014595	6.023360	1.111201
20	1	0	-1.451922	5.914660	0.692564
21	1	0	-2.496594	3.758548	0.221899
22	1	0	-1.310180	-3.484045	-0.815685
23	1	0	-0.175246	-5.590179	-0.180146
24	1	0	1.297655	-5.658549	1.824613
25	1	0	1.599189	-3.606526	3.198643
26	1	0	-3.292015	2.080408	-0.420223
27	1	0	-3.121299	-2.113520	0.382056
28	7	0	0.798156	0.233286	0.332330
29	1	0	1.244508	-0.672888	0.409466
30	6	0	-4.836908	-0.126124	-0.338666
31	6	0	-5.721793	0.879486	0.087617
32	6	0	-5.375560	-1.235127	-1.013889
33	6	0	-7.090875	0.783010	-0.156511
34	1	0	-5.334227	1.731530	0.639294
35	6	0	-6.745029	-1.334846	-1.254595
36	1	0	-4.709365	-2.013942	-1.374886

37	6	0	-7.609901	-0.325246	-0.828390
38	1	0	-7.755114	1.570811	0.189541
39	1	0	-7.135858	-2.199283	-1.785264
40	1	0	-8.677354	-0.401895	-1.016736
41	6	0	0.317451	-2.400583	1.962590
42	1	0	0.438179	-1.514900	2.580795
43	5	0	1.606098	1.378676	0.029897
44	6	0	3.127405	1.039145	-0.373878
45	6	0	3.472711	-0.354984	-0.681952
46	6	0	4.225230	1.917590	-0.315234
47	6	0	2.562962	-1.269861	-1.292657
48	6	0	4.809428	-0.844464	-0.494046
49	6	0	5.550649	1.416164	-0.164579
50	6	0	2.902658	-2.580978	-1.562745
51	1	0	1.590663	-0.915774	-1.612503
52	6	0	5.122864	-2.207627	-0.734283
53	6	0	5.830870	0.078283	-0.155807
54	1	0	6.355981	2.136759	-0.038202
55	6	0	4.183404	-3.075179	-1.241764
56	1	0	2.174423	-3.231648	-2.038569
57	1	0	6.140778	-2.542068	-0.546247
58	1	0	6.842750	-0.282385	0.013972
59	1	0	4.435898	-4.113834	-1.436335
60	6	0	4.171431	3.421316	-0.494635
61	1	0	3.250708	3.757019	-0.968443
62	1	0	4.312510	3.976105	0.442232
63	1	0	5.001641	3.713285	-1.149158

Compound 3 - GS

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -963.549730479 A.U. after 1 cycles
Lowest frequency = 15.7592

Zero-point correction= 0.350108
(Hartree/Particle)
Thermal correction to Energy= 0.368867
Thermal correction to Enthalpy= 0.369812
Thermal correction to Gibbs Free Energy= 0.302183
Sum of electronic and zero-point Energies= -963.199622
Sum of electronic and thermal Energies= -963.180863
Sum of electronic and thermal Enthalpies= -963.179919
Sum of electronic and thermal Free Energies= -963.247548

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.747677	3.422715	-0.777840
2	6	0	-0.095736	2.295914	-0.316000
3	6	0	-0.789973	1.081560	-0.096388
4	6	0	-2.193077	1.024178	-0.363992
5	6	0	-2.828585	2.196670	-0.836294
6	6	0	-2.127877	3.370993	-1.039495
7	6	0	-0.095997	-0.096001	0.389403
8	6	0	-2.917606	-0.221709	-0.148820
9	6	0	-2.199791	-1.359168	0.320422

10	6	0	-0.793659	-1.254939	0.576304
11	6	0	-2.880955	-2.580830	0.532221
12	1	0	-2.314012	-3.437204	0.889907
13	6	0	-4.236119	-2.690680	0.292333
14	6	0	-4.951610	-1.570113	-0.169838
15	6	0	-4.305208	-0.366144	-0.384430
16	1	0	-0.194656	4.343833	-0.940202
17	1	0	0.970478	2.328430	-0.116771
18	1	0	-3.892017	2.184122	-1.048702
19	1	0	-2.647289	4.253330	-1.403629
20	1	0	-0.272912	-2.140186	0.934402
21	1	0	-4.748279	-3.634360	0.458838
22	1	0	-6.018574	-1.649097	-0.360115
23	1	0	-4.886082	0.477600	-0.740770
24	6	0	1.371640	-0.054134	0.696452
25	6	0	2.319712	-0.434505	-0.310200
26	6	0	1.807462	0.335997	1.959671
27	6	0	1.927506	-0.831435	-1.620246
28	6	0	3.720186	-0.415127	-0.001769
29	6	0	3.199781	0.346939	2.240261
30	6	0	2.862991	-1.189242	-2.565091
31	1	0	0.871819	-0.850464	-1.869274
32	6	0	4.659158	-0.793250	-0.999148
33	6	0	4.128687	-0.016498	1.295736
34	1	0	3.527764	0.650450	3.231592
35	6	0	4.244120	-1.172613	-2.254486
36	1	0	2.539246	-1.487399	-3.558805
37	1	0	5.717563	-0.775851	-0.748825
38	1	0	5.190064	-0.001516	1.532743
39	1	0	4.971759	-1.459075	-3.009060
40	6	0	0.833127	0.744786	3.042695
41	1	0	0.213619	1.593018	2.728880
42	1	0	0.145462	-0.070370	3.295764
43	1	0	1.363040	1.034563	3.955270

Compound 3 - TS0

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -963.488272009 A.U. after 1 cycles
Lowest frequency = -33.4862

Zero-point correction= 0.350528
(Hartree/Particle)
Thermal correction to Energy= 0.367898
Thermal correction to Enthalpy= 0.368842
Thermal correction to Gibbs Free Energy= 0.306381
Sum of electronic and zero-point Energies= -963.137744
Sum of electronic and thermal Energies= -963.120374
Sum of electronic and thermal Enthalpies= -963.119430
Sum of electronic and thermal Free Energies= -963.181891

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.679727	3.651904	-0.018425

2	6	0	0.071293	2.419418	-0.183085
3	6	0	0.751475	1.195796	0.017468
4	6	0	2.175524	1.284706	0.193276
5	6	0	2.762321	2.552824	0.410165
6	6	0	2.030421	3.722536	0.344156
7	6	0	0.120868	-0.138058	-0.091184
8	6	0	3.018562	0.110763	0.009421
9	6	0	2.397775	-1.055459	-0.507868
10	6	0	0.971370	-1.129221	-0.537345
11	6	0	3.185507	-2.174522	-0.865463
12	1	0	2.691519	-3.054725	-1.270511
13	6	0	4.554703	-2.162859	-0.679235
14	6	0	5.168339	-1.027484	-0.119053
15	6	0	4.415096	0.085963	0.216253
16	1	0	0.109302	4.559386	-0.197950
17	1	0	-0.936928	2.400018	-0.559699
18	1	0	3.831764	2.618532	0.576634
19	1	0	2.514916	4.682013	0.502458
20	1	0	0.550891	-2.079147	-0.845733
21	1	0	5.153012	-3.028319	-0.950261
22	1	0	6.241940	-1.019748	0.048782
23	1	0	4.919808	0.945527	0.644112
24	6	0	-1.270744	-0.648106	0.223869
25	6	0	-2.560922	0.010828	0.018608
26	6	0	-1.348300	-1.994364	0.651012
27	6	0	-2.825022	1.388421	0.247696
28	6	0	-3.713046	-0.791601	-0.295696
29	6	0	-2.532017	-2.750225	0.427981
30	6	0	-4.054042	1.962182	-0.014056
31	1	0	-2.077988	1.989699	0.740444
32	6	0	-4.947865	-0.173293	-0.625575
33	6	0	-3.643456	-2.200512	-0.148849
34	1	0	-2.523022	-3.803690	0.699028
35	6	0	-5.117176	1.188048	-0.520474
36	1	0	-4.206832	3.015806	0.205009
37	1	0	-5.779961	-0.813235	-0.910336
38	1	0	-4.512487	-2.806713	-0.392108
39	1	0	-6.072518	1.648751	-0.755638
40	6	0	-0.270662	-2.733615	1.431372
41	1	0	0.194582	-3.550854	0.865997
42	1	0	0.526299	-2.076243	1.779426
43	1	0	-0.742676	-3.191477	2.310530

Compound 3 - TS180

Method: b3lyp/6-31g(d)
SCF Done: E(RB3LYP) = -963.489138900 A.U. after 1 cycles
Lowest frequency = -44.0531

Zero-point correction= 0.350843
(Hartree/Particle)
Thermal correction to Energy= 0.368047
Thermal correction to Enthalpy= 0.368991
Thermal correction to Gibbs Free Energy= 0.306909
Sum of electronic and zero-point Energies= -963.138296
Sum of electronic and thermal Energies= -963.121092
Sum of electronic and thermal Enthalpies= -963.120148
Sum of electronic and thermal Free Energies= -963.182230

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.291674	0.368584	0.146145
2	6	0	2.042138	-2.034906	-0.082430
3	6	0	1.891713	1.567434	0.810184
4	6	0	3.681113	0.281101	-0.195955
5	6	0	3.427552	-2.086964	-0.410210
6	6	0	2.751546	2.629558	0.995994
7	1	0	0.890087	1.636664	1.215758
8	6	0	4.530762	1.411894	-0.058190
9	6	0	4.208155	-0.976472	-0.574756
10	1	0	3.868665	-3.073319	-0.537449
11	6	0	4.077264	2.576629	0.513249
12	1	0	2.403731	3.508924	1.531461
13	1	0	5.567311	1.315236	-0.372933
14	1	0	5.249410	-1.059181	-0.875625
15	1	0	4.740352	3.428790	0.634893
16	6	0	1.499859	-3.395469	0.327030
17	1	0	1.234783	-4.045420	-0.517030
18	1	0	0.645629	-3.331855	0.998604
19	1	0	2.298941	-3.913036	0.869939
20	6	0	1.391334	-0.780626	-0.059671
21	6	0	-0.070845	-0.446347	-0.242866
22	6	0	-1.278099	-1.280065	-0.054431
23	6	0	-0.347858	0.836172	-0.674705
24	6	0	-1.317035	-2.669510	-0.302505
25	6	0	-2.536398	-0.651017	0.232934
26	6	0	-1.613524	1.484733	-0.531933
27	1	0	0.455011	1.454398	-1.054646
28	6	0	-2.445841	-3.439809	-0.081195
29	1	0	-0.460897	-3.138092	-0.753469
30	6	0	-3.661109	-1.461874	0.508694
31	6	0	-2.686876	0.789429	0.083344
32	6	0	-1.762556	2.850350	-0.870886
33	6	0	-3.618969	-2.838158	0.391594
34	1	0	-2.421494	-4.504181	-0.299343
35	1	0	-4.604885	-0.989203	0.757598
36	6	0	-3.855442	1.512461	0.405090
37	1	0	-0.932206	3.364615	-1.348970
38	6	0	-2.928871	3.528683	-0.571952
39	1	0	-4.505457	-3.432589	0.594533
40	6	0	-3.974748	2.855597	0.086081
41	1	0	-4.679952	1.020547	0.910358
42	1	0	-3.033418	4.579166	-0.828875
43	1	0	-4.885253	3.390090	0.343269