

Supporting Information:

Aromatic C-F Activation by Complexes Containing the {Pt₂S₂} Core via Nucleophilic Substitution: A Combined Experimental and Theoretical Study

Ainara Nova, Rubén Mas-Ballesté, Gregori Ujaque, Pilar González-Duarte,* Agustí Lledós.*

*Departament de Química, Edifici Cn, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Spain.
Departamento de Química Inorgánica, Universidad Autónoma de Madrid, 28049 Madrid, Spain*

E-mail: Agusti@klingon.uab.es, Pilar.Gonzalez.Duarte@uab.es

Table of Contents

I) Optimized geometries (Cartesian coordinates) for all calculated species	3
II) Experimental details	21
a) Characterization of II	21
b) Characterization of IV	23

I) Optimized Geometries (Cartesian coordinates) and Gas-Phase Energies (hartrees) for all Calculated Species

1

E:	-525.432412		
Pt	-1.646038	0.000044	-0.520642
Pt	1.645912	0.000109	-0.520103
S	0.000015	1.613559	-1.210873
S	0.000071	-1.613168	-1.211384
P	-3.040714	1.700411	0.130143
P	-3.040397	-1.700448	0.130470
P	3.040490	-1.700345	0.130653
P	3.040575	1.700507	0.130658
H	-2.767861	2.314457	1.386836
C	-4.860276	1.306867	0.320008
H	-3.086450	2.877783	-0.664988
H	-3.086067	-2.878068	-0.664305
H	-2.767286	-2.314091	1.387302
C	-4.860016	-1.307167	0.320387
H	3.085761	-2.877936	-0.664179
C	4.860189	-1.307012	0.319710
H	2.768030	-2.314029	1.387618
H	2.768318	2.314297	1.387617
H	3.085843	2.878044	-0.664251
C	4.860255	1.307030	0.319543
H	-5.352331	2.152462	0.814875
H	-5.281583	1.231175	-0.691038
H	-5.281395	-1.231861	-0.690660
H	-5.351881	-2.152711	0.815532
H	5.352324	-2.152571	0.814560
H	5.281069	-1.231623	-0.691538
H	5.281005	1.231441	-0.691743
H	5.352546	2.152606	0.814210
C	5.145723	0.000051	1.102642
C	-5.145248	-0.000064	1.103367
H	-6.208467	-0.000142	1.377643
H	-4.589457	0.000124	2.052587
H	6.209082	0.000037	1.376369
H	4.590419	0.000125	2.052146

C₆F₆

E:	-827.644198		
C	-0.118422	0.000000	1.466204
C	1.085215	0.000000	0.763931
C	1.079347	0.000000	-0.629536
C	-0.130570	0.000000	-1.321015
C	-1.334196	0.000000	-0.618710
F	-2.496230	0.000000	-1.282512
F	-0.137079	0.000000	-2.659759
F	2.235922	0.000000	-1.303309
F	2.247465	0.000000	1.428120
F	-0.112138	0.000000	2.804567
C	-1.328233	0.000000	0.774703
F	-2.484761	0.000000	1.448474

C₅F₅N

E:	-744.467350		
C	21.917542	-0.000011	-26.497142
C	23.155839	-0.000011	-27.134417
C	23.157805	-0.000011	-28.529025
C	21.943264	-0.000011	-29.213944
C	20.779035	-0.000011	-28.449573
F	19.598789	-0.000011	-29.078306
F	21.915357	-0.000011	-30.551245
F	24.308279	-0.000011	-29.198970
F	24.306875	-0.000011	-26.452951
F	21.883398	-0.000011	-25.160507
N	20.768821	-0.000011	-27.135620

1f

E: -1353.092668

Pt	-1.345309	-0.367966	-1.352949
Pt	-0.572006	-0.477862	2.007619
S	-2.550351	-0.868749	0.725334
S	0.442023	-1.406784	-0.026889
P	-3.194758	0.479804	-2.321687
P	-0.149882	-0.025073	-3.365865
P	1.369768	-0.101473	3.244089
P	-1.907236	0.325839	3.658674
H	-4.050804	-0.490333	-2.913189
C	-3.062778	1.743003	-3.679424
H	-4.115515	1.082873	-1.425359
H	1.101600	-0.628858	-3.648461
H	-0.852199	-1.072785	-4.130169
C	-0.679748	1.281891	-4.599002
H	2.603252	0.059946	2.557617
C	1.353442	1.397709	4.355680
H	1.776740	-1.112664	4.162009
H	-2.294335	-0.598734	4.669241
H	-3.179584	0.797829	3.255706
C	-1.225544	1.732225	4.671575
H	-4.083164	1.974485	-4.009146
H	-2.641751	2.653436	-3.233983
H	-0.343249	2.253167	-4.229675
H	-0.138005	1.071104	-5.530119
H	2.288427	1.419451	4.926785
H	1.347323	2.278571	3.701098
H	-1.150242	2.599193	4.002974
H	-1.961293	1.977963	5.446603
C	0.148362	1.447027	5.327652
C	-2.195225	1.292588	-4.881279
H	-2.389129	1.989209	-5.708143
H	-2.521423	0.303095	-5.230845
H	0.340366	2.249693	6.051084
H	0.099573	0.519386	5.916211
C	4.489479	0.531635	-1.142242
C	3.507156	1.316430	-0.547486
C	2.287144	0.751409	-0.194695
C	2.013159	-0.606087	-0.396257
C	3.025990	-1.370350	-0.988064
F	2.837649	-2.682311	-1.218118
F	0.966561	1.292802	-2.583282
F	1.382983	1.557341	0.382711
F	3.743219	2.619351	-0.318206
F	5.669283	1.070806	-1.483403
C	4.248212	-0.820244	-1.363344
F	5.197572	-1.587672	-1.926223

2f

E:	-1353.095931		
Pt	-0.075165	-0.136766	1.699062
Pt	-0.970561	-0.068109	-1.476223
S	-0.285657	-1.816317	-0.011764
S	0.694015	1.328039	-0.261951
P	-0.976857	-1.483467	3.349836
P	0.238990	1.476199	3.324510
P	-1.622516	1.665248	-2.895826
P	-2.492890	-1.562540	-2.229387
H	-2.069374	-2.036575	2.574072
C	-2.063799	-0.759054	4.687536
H	-0.442992	-2.748482	3.686298
H	1.527958	1.529566	3.904530
H	0.178879	2.806345	2.808241
C	-0.924866	1.581473	4.785053
H	-0.618478	2.525080	-3.418481
C	-2.544368	1.181642	-4.446891
H	-2.487221	2.665743	-2.363062
H	-3.661896	-1.675082	-1.432250
H	-2.079497	-2.916323	-2.261859
C	-3.204443	-1.292867	-3.932587
H	-3.049794	-1.231933	4.609214
H	-1.617485	-1.023164	5.649917
H	-0.377811	1.203286	5.652902
H	-1.159870	2.638864	4.953191
H	-2.951166	2.089414	-4.906364
H	-1.804643	0.768110	-5.144460
H	-2.428107	-1.577738	-4.654534
H	-4.039594	-1.991938	-4.061467
C	-3.680591	0.154100	-4.215096
C	-2.231312	0.775782	4.593594

H	-2.937008	1.086636	5.376795
H	-2.696840	1.040319	3.633753
H	-4.295960	0.129613	-5.123508
H	-4.346880	0.498729	-3.410994
C	4.846428	-0.287754	-1.510094
C	4.566097	-0.006631	-0.176833
C	3.308337	0.469095	0.182580
C	2.285572	0.665895	-0.755323
C	2.614743	0.402855	-2.090286
F	1.720707	0.626838	-3.075312
F	0.504544	-0.889998	4.512007
F	3.107716	0.760225	1.477868
F	5.515727	-0.182613	0.755325
F	6.057302	-0.740342	-1.867889
C	3.863629	-0.076061	-2.471109
F	4.129219	-0.319781	-3.766980

3f

E:	-1353.111375		
Pt	0.202999	-0.160587	1.746311
Pt	-0.423642	-0.147953	-1.390973
S	0.412224	-2.006513	0.018217
S	1.431136	0.988939	-0.073374
P	-0.875032	-1.343226	3.374330
P	0.121422	1.673213	3.171040
P	-1.047750	1.608583	-2.705425
P	-2.089200	-1.400657	-2.419453
H	-1.690265	-2.375649	2.829157
C	-2.033492	-0.488400	4.560572
H	-0.020377	-2.120859	4.188457
H	1.278002	2.372843	3.582827
H	-0.214063	2.653019	2.143188
C	-1.382184	2.011600	4.224234
H	-0.228693	1.798134	-3.842807
C	-2.794700	1.736665	-3.348306
H	-0.854456	2.862151	-2.059474
H	-2.573335	-2.012977	-1.184573
H	-1.843406	-2.648766	-3.035949
C	-3.732754	-0.642545	-2.875371
H	-2.910655	-1.134356	4.682317
H	-1.511282	-0.424181	5.518870
H	-1.045331	2.083828	5.261880
H	-1.801196	2.976591	3.918414
H	-3.083550	2.792890	-3.301659
H	-2.766931	1.428105	-4.396931
H	-3.887666	-0.813431	-3.944002
H	-4.514989	-1.165534	-2.314203
C	-3.814523	0.871662	-2.569923
C	-2.475764	0.922718	4.103733
H	-3.324391	1.226727	4.731226
H	-2.853653	0.883756	3.072422
H	-4.821557	1.217191	-2.839571
H	-3.709080	1.042343	-1.489188
C	4.416014	-2.450354	-0.771875
C	4.859802	-1.138817	-0.820294
C	3.953104	-0.092405	-0.608734
C	2.615478	-0.348572	-0.350800
C	2.162357	-1.683965	-0.306746
F	-1.463967	-0.722435	-4.109253
F	0.660523	0.473391	4.601623
F	4.423381	1.168050	-0.663347
F	6.151276	-0.871711	-1.067147
F	5.275095	-3.461405	-0.971606
C	3.064792	-2.715366	-0.514470
F	2.671971	-4.002474	-0.477351

4f

E:	-900.840847		
Pt	-0.383222	-0.208815	-1.611498
S	0.653670	-2.270138	-1.101587
S	1.735443	0.836826	-1.565505
P	-1.349711	1.823136	-2.145670
P	-2.430699	-1.281572	-1.684050
H	-0.492770	2.796862	-2.722097
C	-2.788062	1.775251	-3.330028
H	-1.889470	2.596233	-1.079096
H	-3.230467	-1.254784	-0.506652
H	-2.400692	-2.682989	-1.907412

C	-3.641986	-0.677671	-2.965433
H	-3.167992	2.796201	-3.450420
H	-2.394414	1.453596	-4.302275
H	-3.223823	-0.929161	-3.948070
H	-4.574030	-1.242645	-2.850198
C	-3.940407	0.840622	-2.883261
H	-4.799438	1.042750	-3.535334
H	-4.267283	1.105405	-1.867470
C	4.640709	-2.529132	-0.443065
C	5.094719	-1.225110	-0.637651
C	4.186930	-0.232616	-0.975224
C	2.819727	-0.498886	-1.126204
C	2.361405	-1.815263	-0.929741
F	4.651427	1.024086	-1.159264
F	6.403913	-0.940842	-0.495950
F	5.512109	-3.502309	-0.113727
C	3.290329	-2.807861	-0.590931
F	2.874362	-4.080068	-0.397576

[PtF₂(dhpp)]

E:	-452.260540		
Pt	-0.135027	-0.328809	-0.005289
P	-1.614479	-1.533956	1.163011
P	-0.711840	1.710006	0.713348
H	-2.669352	-2.086612	0.389072
C	-2.513089	-0.680281	2.552095
H	-1.097987	-2.708373	1.764470
H	0.369917	2.567559	1.033049
H	-1.391996	2.504858	-0.247281
C	-1.818906	1.813858	2.206467
H	-3.382819	-1.289149	2.824818
H	-1.840229	-0.671785	3.419274
H	-1.184342	1.684436	3.092690
H	-2.237521	2.825774	2.254696
C	-2.963526	0.767388	2.225007
H	-3.680698	1.073934	2.996661
H	-3.514908	0.789145	1.274559
F	0.412012	-2.138526	-0.707114
F	1.203880	0.706454	-1.101691

TS1f

E:	-1353.044371		
Pt	-0.584676	-0.288416	-2.190760
Pt	-1.250207	-0.316847	1.324979
S	-2.244788	0.533268	-0.671992
S	0.298096	-1.375744	-0.218063
P	-1.327193	1.089225	-3.855395
P	1.067118	-1.106330	-3.608545
P	-0.334418	-1.256118	3.254196
P	-2.664285	0.966081	2.598874
H	-2.032600	0.566292	-4.978153
C	0.062019	2.022002	-4.675586
H	-2.230300	2.110567	-3.461351
H	2.071114	-1.952349	-3.084596
H	0.627153	-1.892295	-4.715197
C	2.000081	0.238880	-4.496888
H	0.882037	-1.977565	3.174436
C	-0.052699	-0.080987	4.673758
H	-1.140504	-2.248823	3.883063
H	-3.844553	0.371926	3.131309
H	-3.238749	2.080054	1.934771
C	-1.895973	1.712356	4.123593
H	-0.369435	2.730008	-5.393081
H	0.551388	2.603435	-3.884585
H	2.489248	0.841858	-3.722817
H	2.786762	-0.218015	-5.108246
H	0.357516	-0.644819	5.519108
H	0.716439	0.631078	4.350538
H	-1.095568	2.380860	3.782596
H	-2.651877	2.329292	4.623344
C	-1.329964	0.671641	5.124610
C	1.099217	1.122716	-5.398362
H	1.759760	1.788074	-5.969206
H	0.589331	0.494895	-6.143584
H	-1.083925	1.209853	6.048793
H	-2.114012	-0.049894	5.396955
C	3.094976	1.105930	2.467873
C	2.455579	1.747774	1.406932

C	1.934757	1.035099	0.343085
C	1.997740	-0.389908	0.227979
C	2.666223	-0.991197	1.337332
F	2.737497	-2.355253	1.386203
F	2.686269	-0.779381	-1.130434
F	1.325870	1.739872	-0.650534
F	2.344096	3.096978	1.421834
F	3.629929	1.809504	3.501243
C	3.190943	-0.280744	2.406287
F	3.780141	-0.954403	3.424031

TS2f

E: -1353,03945687

Pt	-0.591636	-0.001530	1.552366
Pt	-0.655417	0.085156	-1.668609
S	0.335824	-1.517524	-0.117536
S	0.442652	1.592155	-0.083435
P	-1.560834	-1.654725	2.880683
P	-1.404360	1.532948	3.053063
P	-1.347578	1.740098	-3.103194
P	-1.351767	-1.594660	-3.067798
H	-2.046635	-2.512535	1.808865
C	-3.238520	-1.381713	3.656913
H	-0.817183	-2.687139	3.494587
H	-0.480745	1.954640	4.035710
H	-1.678816	2.792216	2.442181
C	-2.991234	1.195215	3.977949
H	-0.723854	3.005555	-2.951308
C	-1.099919	1.367113	-4.910882
H	-2.711397	2.146506	-3.066285
H	-2.714633	-2.001230	-3.027809
H	-0.709274	-2.839394	-2.860813
C	-1.086369	-1.254574	-4.876957
H	-3.926504	-2.133657	3.254203
H	-3.127905	-1.541675	4.732748
H	-2.712247	0.975522	5.011765
H	-3.584499	2.116929	3.961844
H	-1.494987	2.207349	-5.493248
H	-0.016224	1.329711	-5.078928
H	-0.000390	-1.207485	-5.026412
H	-1.461029	-2.112129	-5.447646
C	-1.756454	0.046335	-5.386210
C	-3.820770	0.027199	3.393689
H	-4.820645	0.068049	3.847391
H	-3.965223	0.174135	2.313903
H	-1.705977	0.033691	-6.482175
H	-2.827489	0.044524	-5.136851
C	4.354526	-0.643841	0.524539
C	4.304488	0.726179	0.806108
C	3.140197	1.407845	0.492547
C	2.055609	0.779277	-0.118580
C	2.126275	-0.598668	-0.501452
F	1.951289	-0.833794	-2.061868
F	-0.888575	-0.648994	4.441972
F	3.040945	2.715530	0.842370
F	5.370019	1.356063	1.359576
F	5.465749	-1.338468	0.840815
C	3.299440	-1.286958	-0.091114
F	3.385001	-2.624958	-0.319517

1n

E: -1269.915347

Pt	-0.650540	-0.572868	1.914180
Pt	-1.018535	-0.422186	-1.527367
S	0.618054	-1.457317	-0.001599
S	-2.458478	-0.929919	0.394306
P	1.123898	-0.237812	3.395152
P	-2.187118	0.158952	3.414341
P	-2.742174	0.420052	-2.705377
P	0.399536	-0.079999	-3.390806
H	1.436267	-1.296463	4.296066
C	0.949963	1.194778	4.577712
H	2.427657	-0.023220	2.872198
H	-3.396561	0.657419	2.873456
H	-2.699791	-0.820914	4.309804
C	-1.650764	1.503216	4.586207
H	-3.763907	1.016338	-1.921171

C	-2.451494	1.688185	-4.033571
H	-3.516255	-0.552902	-3.396344
H	-0.216347	-1.124298	-4.230503
H	1.672422	-0.689478	-3.527659
C	0.021053	1.228357	-4.675442
H	1.806232	1.188460	5.261450
H	1.014883	2.111752	3.978388
H	-1.501067	2.409999	3.986513
H	-2.481079	1.699001	5.275156
H	-3.426929	1.922394	-4.477634
H	-2.083539	2.595987	-3.538676
H	0.315864	2.198837	-4.270099
H	0.665647	1.015595	-5.538018
C	-1.451684	1.241339	-5.129557
C	-0.367457	1.182592	5.392394
H	-0.275426	1.941291	6.179982
H	-0.480524	0.221515	5.914790
H	-1.549577	1.941210	-5.970422
H	-1.735829	0.253406	-5.517899
C	4.509091	-0.642157	-0.830620
C	3.296743	-1.302098	-0.655328
C	2.188197	-0.598111	-0.169273
C	2.402770	0.755835	0.107980
C	3.664569	1.303371	-0.093688
F	3.863916	2.598865	0.204625
F	1.422392	1.536614	0.586396
F	1.415589	1.227911	-2.477308
F	3.202625	-2.609046	-0.957535
F	5.564836	-1.330430	-1.297888
N	4.693568	0.627270	-0.550365

2n

E:	-1269.919862		
Pt	-0.545749	0.186695	1.839283
Pt	-0.448637	0.262780	-1.484114
S	0.707607	-1.258676	0.245636
S	-0.201521	1.920971	0.242378
P	-0.874196	-1.516656	3.398945
P	-1.804632	1.734787	2.902252
P	-1.690290	1.665948	-2.839106
P	-0.533576	-1.307806	-3.175379
H	-1.836396	-2.519570	3.083335
C	-1.436015	-0.998679	5.103713
H	0.218066	-2.373197	3.705904
H	-1.332981	3.068170	2.847108
H	-3.106534	1.899540	2.363364
C	-2.153134	1.481074	4.717476
H	-1.263750	2.966970	-3.192783
C	-3.045127	1.000087	-3.943022
H	-2.595747	2.138349	-1.807665
H	-0.521565	-2.654149	-2.702795
H	0.604841	-1.362143	-4.014039
C	-1.967750	-1.330178	-4.375754
H	-1.745661	-1.893904	5.654280
H	-0.559331	-0.586711	5.619828
H	-1.241068	1.756192	5.262835
H	-2.932688	2.194862	5.010130
H	-3.986889	1.467108	-3.631974
H	-2.815773	1.308874	-4.966336
H	-1.600467	-0.904911	-5.313948
H	-2.240832	-2.377021	-4.552376
C	-3.201983	-0.538037	-3.885262
C	-2.582461	0.043612	5.102004
H	-2.997784	0.081458	6.117097
H	-3.404263	-0.294125	4.454115
H	-4.054717	-0.813982	-4.521284
H	-3.465548	-0.847604	-2.864061
C	4.392906	0.031319	1.470569
C	3.061525	-0.365112	1.506295
C	2.396410	-0.686039	0.315445
C	3.183689	-0.616312	-0.843158
C	4.510441	-0.209016	-0.756197
F	5.244225	-0.145027	-1.878153
F	2.679143	-0.960373	-2.039726
F	-0.500819	1.176266	-4.297798
F	2.441242	-0.456748	2.699902
F	5.007265	0.340830	2.626516
N	5.105931	0.112347	0.370740

3n

E:	-1269.933860		
Pt	-0.396660	-0.079663	1.581521
Pt	-0.155531	-0.074878	-1.612906
S	1.012673	-1.593440	0.078118
S	0.649885	1.564912	0.055606
P	-1.223594	-1.670984	2.996268
P	-1.616044	1.483333	2.790678
P	-1.191305	1.490063	-2.981332
P	-0.765830	-1.662320	-3.138148
H	-1.343075	-2.940509	2.361065
C	-2.896516	-1.453445	3.793778
H	-0.350540	-2.018426	4.052214
H	-1.022640	2.609089	3.404664
H	-2.068020	2.236958	1.628674
C	-3.326814	1.090218	3.420709
H	-0.519101	2.618002	-3.503240
C	-2.794667	1.095016	-3.848639
H	-1.805435	2.240976	-1.894374
H	-0.968755	-2.935380	-2.531812
H	0.249373	-2.001460	-4.061256
C	-2.310386	-1.446900	-4.162742
H	-3.408421	-2.421584	3.748657
H	-2.716372	-1.201988	4.842406
H	-3.327079	1.268640	4.499272
H	-4.030838	1.781887	2.944946
H	-3.560528	1.784195	-3.475941
H	-2.642524	1.276088	-4.915970
H	-1.985373	-1.193253	-5.175339
H	-2.821234	-2.416222	-4.191482
C	-3.272374	-0.360015	-3.626108
C	-3.770997	-0.363316	3.129227
H	-4.796736	-0.483771	3.502897
H	-3.816358	-0.528732	2.043976
H	-4.234737	-0.481491	-4.141276
H	-3.470236	-0.528107	-2.558511
C	3.465117	1.626028	0.275392
C	2.310957	0.861735	0.183431
C	2.465492	-0.540826	0.194475
C	3.750021	-1.055149	0.296520
C	4.823494	-0.160604	0.382585
F	6.065199	-0.659091	0.481063
F	3.981086	-2.381095	0.314132
F	-0.342494	0.614406	-4.487996
F	-0.991097	0.603549	4.400088
F	3.371499	2.967759	0.268301
N	4.693458	1.140637	0.372835

4n

E:	-1269.904584		
Pt	-1.122117	-0.520760	-1.741416
Pt	-0.719574	-0.173373	1.695863
S	-2.590696	-0.495922	0.143429
S	0.428898	-1.439103	-0.075260
P	-2.853015	0.314446	-2.956176
P	0.314750	-0.596231	-3.577576
P	1.103339	-0.038659	3.199241
P	-2.013581	0.949732	3.158394
H	-3.728409	-0.648567	-3.530801
C	-2.437367	1.378719	-4.428386
H	-3.789779	1.101965	-2.244621
H	1.716054	-0.485774	-3.364308
H	0.323332	-1.793482	-4.349840
C	0.037049	0.680657	-4.910027
H	2.301484	-0.777543	3.043997
C	1.186124	1.261267	4.543059
H	0.575383	-1.032712	4.149726
H	-2.810317	0.125495	4.000907
H	-3.039429	1.733604	2.568293
C	-1.257394	2.123452	4.385666
H	-3.373227	1.607652	-4.952006
H	-2.041535	2.325355	-4.038962
H	0.335939	1.650086	-4.491310
H	0.709316	0.463260	-5.747605
H	1.935870	0.915450	5.266318
H	1.550575	2.189793	4.098632
H	-0.839400	2.963057	3.815942

H	-2.071359	2.514128	5.008677
C	-0.155554	1.485513	5.269390
C	-1.425114	0.748877	-5.416919
H	-1.431761	1.358458	-6.329477
H	-1.766718	-0.250838	-5.722154
H	0.018934	2.159149	6.119182
H	-0.515809	0.539440	5.697559
C	4.317394	-1.073603	0.039122
C	4.666445	0.218431	-0.348434
C	3.629324	1.063870	-0.717654
C	2.317953	0.596177	-0.669606
C	2.072489	-0.716854	-0.265533
F	2.035614	1.191825	2.072411
F	1.338950	1.440754	-1.024891
F	3.887534	2.315449	-1.110883
F	5.940436	0.635942	-0.383668
F	5.302206	-1.920736	0.390636
N	3.090229	-1.521234	0.071217

5n

E: -817.666142

Pt	-0.381356	-0.193848	-1.606569
S	0.656912	-2.258905	-1.108785
S	1.741091	0.858151	-1.545574
P	-1.359481	1.833739	-2.146677
P	-2.422136	-1.275320	-1.676229
H	-0.508361	2.810633	-2.726358
C	-2.793417	1.770076	-3.334845
H	-1.905657	2.608400	-1.084571
H	-3.217953	-1.242585	-0.496825
H	-2.382556	-2.677758	-1.889948
C	-3.636318	-0.684880	-2.960611
H	-3.178197	2.788186	-3.463333
H	-2.394117	1.444306	-4.303397
H	-3.217435	-0.939747	-3.942087
H	-4.565193	-1.254296	-2.841644
C	-3.942754	0.832293	-2.886925
H	-4.800461	1.026808	-3.542955
H	-4.274300	1.100735	-1.873644
N	4.617628	-2.525484	-0.461842
C	5.030832	-1.286132	-0.637651
C	4.190189	-0.236604	-0.965644
C	2.816391	-0.475026	-1.123659
C	2.359908	-1.793833	-0.938011
F	4.689632	1.008727	-1.130433
F	6.349289	-1.050276	-0.483482
C	3.332956	-2.747407	-0.611683
F	2.933033	-4.026539	-0.428281

TS1n

E: -1269.88351955

Pt	1.436135	-1.135929	-0.456760
Pt	-2.095200	-0.588130	-0.451604
S	-0.130560	0.488541	-1.383158
S	-0.553541	-2.347968	0.067036
P	3.383545	0.007726	-1.072877
P	2.694928	-2.605794	0.761587
P	-3.735694	-1.513917	0.828474
P	-3.548145	1.164600	-0.967759
H	4.210413	-0.668031	-2.016469
C	4.592334	0.302164	0.315162
H	3.292364	1.266642	-1.715381
H	1.974781	-3.412236	1.679205
H	3.445864	-3.612230	0.088753
C	3.998523	-1.787685	1.810331
H	-3.355067	-2.605759	1.650998
C	-4.431748	-0.269852	2.028680
H	-4.914084	-2.053196	0.235723
H	-4.732628	0.780013	-1.666746
H	-3.119606	2.241990	-1.771962
C	-4.289976	1.922980	0.560163
H	5.460947	0.837887	-0.084266
H	4.100834	0.970171	1.033412
H	3.473013	-1.117360	2.501645
H	4.491126	-2.562118	2.410092
H	-5.121795	-0.788169	2.705113
H	-3.582116	0.086783	2.623855
H	-3.448349	2.290594	1.157458

H	-4.897629	2.788525	0.272462
C	-5.163316	0.930335	1.369458
C	5.067128	-1.000705	1.006816
H	5.861892	-0.724512	1.711212
H	5.538053	-1.664340	0.266996
H	-5.637981	1.498055	2.180202
H	-5.985743	0.560876	0.739945
C	2.177619	3.400302	0.113098
C	1.263129	2.808269	-0.729792
C	0.228521	1.951355	-0.234342
C	0.366771	1.746330	1.178672
C	1.330904	2.401264	1.906654
F	1.388379	2.173346	3.244356
F	-0.513789	0.931686	1.823007
F	-1.257644	2.704546	-0.471963
F	1.340366	3.032605	-2.073730
F	3.128965	4.198616	-0.434699
N	2.251859	3.218410	1.419216

TS2n

E: -1269.86090491

Pt	1.580735	-0.716804	-0.116156
Pt	-1.621138	-0.254807	0.007587
S	0.137541	0.660335	-1.542480
S	0.155461	0.330542	1.564468
P	2.938861	-1.458699	-1.815183
P	2.912145	-1.631576	1.510499
P	-3.048774	-1.165987	1.607044
P	-3.241436	-0.713904	-1.553528
H	2.787269	-2.797037	-2.275981
C	4.762652	-1.375153	-1.446667
H	2.832557	-0.772780	-3.053014
H	2.753054	-1.048569	2.790533
H	2.767284	-3.009723	1.833161
C	4.734407	-1.483650	1.173717
H	-3.514390	-0.444075	2.728739
C	-4.064341	-2.684767	1.215327
H	-2.035615	-1.881209	2.371284
H	-2.700384	-0.961594	-2.849142
H	-4.084879	0.376743	-1.863309
C	-4.386759	-2.170659	-1.320416
H	5.307125	-1.777917	-2.308390
H	5.017710	-0.311225	-1.362871
H	4.961839	-0.410352	1.178320
H	5.277601	-1.940410	2.009076
H	-3.753763	-3.485614	1.895796
H	-5.110653	-2.436800	1.412664
H	-5.363321	-1.763608	-1.045262
H	-4.477550	-2.677394	-2.288139
C	-3.908418	-3.173826	-0.244030
C	5.189825	-2.126523	-0.160431
H	6.286525	-2.157926	-0.151527
H	4.861593	-3.174997	-0.208046
H	-4.500241	-4.092662	-0.356215
H	-2.862515	-3.454756	-0.432139
C	0.510550	3.331161	1.468886
C	0.765354	2.124383	0.754964
C	0.372497	2.190803	-0.612460
C	-0.063671	3.403724	-1.151939
C	-0.170899	4.513925	-0.334076
F	-0.564685	5.708036	-0.845183
F	-0.430236	3.470550	-2.456239
F	-4.503895	-0.189774	0.729999
F	2.296804	1.735771	0.989452
F	0.706258	3.302263	2.814396
N	0.088110	4.452557	0.958497

TS3n

scf done: -1353.044371

Pt	-0.584676	-0.288416	-2.190760
Pt	-1.250207	-0.316847	1.324979
S	-2.244788	0.533268	-0.671992
S	0.298096	-1.375744	-0.218063
P	-1.327193	1.089225	-3.855395
P	1.067118	-1.106330	-3.608545
P	-0.334418	-1.256118	3.254196
P	-2.664285	0.966081	2.598874
H	-2.032600	0.566292	-4.978153

C	0.062019	2.022002	-4.675586
H	-2.230300	2.110567	-3.461351
H	2.071114	-1.952349	-3.084596
H	0.627153	-1.892295	-4.715197
C	2.000081	0.238880	-4.496888
H	0.882037	-1.977565	3.174436
C	-0.052699	-0.080987	4.673758
H	-1.140504	-2.248823	3.883063
H	-3.844553	0.371926	3.131309
H	-3.238749	2.080054	1.934771
C	-1.895973	1.712356	4.123593
H	-0.369435	2.730008	-5.393081
H	0.551388	2.603435	-3.884585
H	2.489248	0.841858	-3.722817
H	2.786762	-0.218015	-5.108246
H	0.357516	-0.644819	5.519108
H	0.716439	0.631078	4.350538
H	-1.095568	2.380860	3.782596
H	-2.651877	2.329292	4.623344
C	-1.329964	0.671641	5.124610
C	1.099217	1.122716	-5.398362
H	1.759760	1.788074	-5.969206
H	0.589331	0.494895	-6.143584
H	-1.083925	1.209853	6.048793
H	-2.114012	-0.049894	5.396955
C	3.094976	1.105930	2.467873
C	2.455579	1.747774	1.406932
C	1.934757	1.035099	0.343085
C	1.997740	-0.389908	0.227979
C	2.666223	-0.991197	1.337332
F	2.737497	-2.355253	1.386203
F	2.686269	-0.779381	-1.130434
F	1.325870	1.739872	-0.650534
F	2.344096	3.096978	1.421834
F	3.629929	1.809504	3.501243
C	3.190943	-0.280744	2.406287
F	3.780141	-0.954403	3.424031

T

scf done: -977.746086

Pt	-1.783097	-0.571707	-0.041477
Pt	0.672344	1.703289	0.040269
S	0.101005	-0.050713	-1.567815
S	0.011638	-0.137351	1.564186
P	-3.364080	-0.984509	-1.651576
P	-3.420879	-1.058574	1.533866
P	1.206533	3.242840	1.654514
P	1.279521	3.303012	-1.532378
H	-3.100671	-0.225791	-2.832965
C	-5.154294	-0.556510	-1.333439
H	-3.380184	-2.275188	-2.225867
H	-3.365821	-2.195293	2.370103
H	-3.087686	-0.120885	2.587304
C	-5.175966	-0.472882	1.276133
H	2.495107	3.156534	2.227604
C	0.920715	5.062145	1.341746
H	0.430892	3.036076	2.836125
H	0.314488	3.048846	-2.582888
H	2.405511	3.162732	-2.373233
C	0.837211	5.098110	-1.266539
H	-5.523564	-0.005706	-2.206805
H	-5.693517	-1.503986	-1.256669
H	-5.818258	-1.356657	1.304768
H	-5.440441	0.189484	2.108652
H	0.402563	5.471638	2.217120
H	1.907668	5.524996	1.263653
H	1.769493	5.667770	-1.291443
H	0.198628	5.418699	-2.097942
C	0.096725	5.357430	0.066604
C	-5.382616	0.285565	-0.056208
H	-6.419727	0.649167	-0.078055
H	-4.741706	1.178270	-0.078568
H	-0.188671	6.418593	0.091856
H	-0.840473	4.783970	0.087948
F	2.842512	3.781011	-0.225485
F	-4.025407	-2.570246	0.225548
Pt	1.323616	-1.453167	-0.003173
P	2.424660	-2.541123	-1.697930
P	2.326411	-2.635887	1.688771

H	2.783248	-1.768274	-2.833014
C	4.025422	-3.406271	-1.285893
H	1.697317	-3.574266	-2.352324
H	1.560699	-3.700006	2.241227
H	2.619168	-1.929724	2.884733
C	3.948453	-3.482567	1.323879
H	4.312784	-4.023929	-2.144551
H	4.792101	-2.628806	-1.173201
H	4.721600	-2.703677	1.303166
H	4.182760	-4.150680	2.160626
C	3.967089	-4.277543	-0.005944
H	4.859640	-4.916032	0.001750
H	3.108649	-4.963335	-0.050924

Endo

E: -1169,8864986

Pt	-0.04004	-0.00890	-0.04314
Pt	1.82058	-2.84806	0.56034
S	-0.21260	-2.37383	-0.76411
S	2.25541	-0.62947	-0.22278
C	-2.42511	2.42371	-0.83690
C	-1.77304	3.47555	0.09490
C	-0.22914	3.53074	0.02786
C	2.80505	-6.18273	1.16327
C	4.06923	-5.75611	1.94670
C	4.82486	-4.53411	1.37365
H	-3.48011	2.66747	-0.99477
H	-1.94236	2.43965	-1.82159
H	-2.11002	3.33614	1.13151
H	-2.14487	4.46173	-0.20713
H	0.14143	4.42366	0.54260
H	0.08925	3.61555	-1.01890
H	2.49028	-7.18027	1.48679
H	3.02100	-6.24172	0.08959
H	3.81839	-5.60296	3.00396
H	4.76849	-6.60070	1.92872
H	5.79296	-4.41974	1.87496
H	5.04094	-4.70682	0.31082
C	-1.70226	-3.12335	-0.09225
C	-2.07513	-3.10618	1.25669
C	-3.28785	-3.67304	1.64086
N	-4.11705	-4.25455	0.80424
C	-3.77333	-4.30966	-0.46320
C	-2.59073	-3.76590	-0.96561
F	-2.31879	-3.86009	-2.27370
F	-1.27612	-2.56097	2.18820
F	-3.63723	-3.63282	2.93198
F	-4.61275	-4.91846	-1.30368
P	-2.28820	0.68188	-0.18426
P	0.64731	2.03851	0.70736
P	3.95205	-2.88672	1.41305
P	1.38477	-4.99680	1.37578
C	-3.32702	0.77684	1.31687
C	-3.30819	-0.28764	-1.35098
C	2.42146	2.38752	0.43875
C	0.44598	2.07971	2.52377
C	5.12790	-1.84815	0.47480
C	4.04320	-2.23146	3.11714
C	1.13846	-5.01652	3.18700
C	-0.04167	-5.91491	0.69466
C	-4.47170	-0.96336	-0.96960
C	-5.21342	-1.67591	-1.91410
C	-4.78490	-1.73573	-3.24075
C	-3.61304	-1.08079	-3.62191
C	-2.87741	-0.35966	-2.67960
H	-4.81743	-0.95295	0.07603
H	-6.13302	-2.20333	-1.60848
H	-5.36467	-2.30914	-3.98360
H	-3.26468	-1.13727	-4.66701
H	-1.94866	0.14722	-2.99104
C	-2.83002	0.22911	2.49992
C	-3.58383	0.27005	3.67327
C	-4.84729	0.86232	3.66870
C	-5.35147	1.41241	2.48895
C	-4.59392	1.36998	1.31634
H	-5.01171	1.80182	0.39238
H	-6.35083	1.87970	2.48254
H	-5.44529	0.89568	4.59509
H	-3.17847	-0.16464	4.60255

H	-1.83460	-0.23665	2.51224
C	3.33354	2.45584	1.49703
C	4.68472	2.70425	1.24775
C	5.13231	2.89026	-0.06089
C	4.22647	2.82663	-1.12045
C	2.87550	2.57716	-0.87110
H	2.17260	2.51220	-1.71849
H	4.57965	2.96236	-2.15667
H	6.20112	3.07870	-0.25835
H	5.40063	2.74529	2.08613
H	3.00423	2.30486	2.53718
C	0.44678	0.85222	3.19303
C	0.29214	0.80459	4.57922
C	0.15316	1.98826	5.30527
C	0.17201	3.21709	4.64246
C	0.32102	3.26343	3.25439
H	0.34056	4.24106	2.74737
H	0.06752	4.15362	5.21610
H	0.03121	1.95286	6.40108
H	0.28198	-0.16874	5.09824
H	0.56262	-0.08762	2.62741
C	5.14995	-1.97632	-0.91838
C	6.02944	-1.20879	-1.68434
C	6.90553	-0.31983	-1.06010
C	6.90650	-0.20797	0.33104
C	6.02465	-0.97363	1.09666
H	6.05190	-0.87784	2.19370
H	7.60545	0.48637	0.82748
H	7.59950	0.28854	-1.66447
H	6.03056	-1.30502	-2.78329
H	4.46429	-2.67908	-1.42157
C	4.56765	-2.96469	4.18529
C	4.59929	-2.41761	5.46989
C	4.11349	-1.12909	5.69525
C	3.59378	-0.38970	4.63280
C	3.55225	-0.94297	3.35207
H	3.13559	-0.35041	2.52310
H	3.21477	0.63178	4.80447
H	4.14179	-0.69583	6.70934
H	5.00976	-3.00590	6.30804
H	4.96001	-3.98132	4.03292
C	1.05703	-3.78672	3.84541
C	0.88818	-3.73876	5.22980
C	0.79640	-4.92333	5.96234
C	0.87737	-6.15431	5.30827
C	1.05170	-6.20142	3.92340
H	1.12107	-7.17983	3.42007
H	0.80839	-7.09106	5.88692
H	0.66456	-4.88638	7.05697
H	0.83524	-2.76410	5.74347
H	1.13704	-2.84654	3.27541
C	-1.14034	-6.30085	1.46826
C	-2.19417	-7.01074	0.88895
C	-2.16253	-7.32670	-0.47000
C	-1.07598	-6.92892	-1.25000
C	-0.01936	-6.22535	-0.66893
H	-1.19736	-6.04462	2.53791
H	-3.05948	-7.31129	1.50374
H	-3.00001	-7.87893	-0.92879
H	-1.05419	-7.16559	-2.32715
H	0.83091	-5.91040	-1.29683

Exo(A)

E: -1169,88321715

Pt	2.12256	0.32296	-1.09385
Pt	-0.37658	2.29081	-2.36931
S	0.32919	1.73340	-0.07400
S	1.86198	1.72085	-3.00256
C	3.90854	-2.10996	0.90045
C	4.25549	-2.88771	-0.39187
C	4.69388	-2.02174	-1.59983
C	-3.71868	3.60204	-2.76043
C	-3.61589	3.10900	-4.22645
C	-2.35097	3.59533	-4.98000
H	3.78337	-2.80979	1.73398
H	4.75104	-1.45660	1.16380
H	3.43166	-3.54902	-0.68807
H	5.09229	-3.55270	-0.14629
H	5.17212	-2.65731	-2.35376

H	5.43077	-1.27149	-1.28939
H	-4.74028	3.46767	-2.39188
H	-3.50492	4.67667	-2.71909
H	-3.70007	2.01412	-4.27398
H	-4.48957	3.49792	-4.76215
H	-2.51895	3.55162	-6.06119
H	-2.14954	4.64472	-4.73233
C	0.93126	3.20574	0.75185
C	0.79830	3.25635	2.14876
C	1.19230	4.39720	2.84043
N	1.69250	5.46159	2.25538
C	1.81730	5.43800	0.94861
C	1.46252	4.35212	0.14758
F	1.61914	4.44473	-1.17618
F	0.28689	2.21425	2.82746
F	1.05668	4.42634	4.17018
F	2.31331	6.52987	0.35727
P	2.42672	-0.96803	0.85143
P	3.27215	-1.13437	-2.39915
P	-0.81480	2.62697	-4.57806
P	-2.53062	2.75002	-1.60383
C	0.94584	-1.93897	1.30514
C	2.77261	0.03882	2.33743
C	3.85035	-0.47565	-4.00332
C	2.16042	-2.51512	-2.84543
C	0.56630	3.51698	-5.37933
C	-0.99875	1.07243	-5.52207
C	-3.40002	1.22913	-1.08172
C	-2.46611	3.77680	-0.09283
C	2.43638	-0.37338	3.62901
C	2.73884	0.44039	4.72309
C	3.39757	1.65663	4.53106
C	3.76228	2.05577	3.24400
C	3.45149	1.24668	2.14948
H	1.93502	-1.34069	3.79654
H	2.46221	0.11878	5.74141
H	3.63710	2.29758	5.39638
H	4.29593	3.00940	3.09225
H	3.74700	1.56380	1.13486
C	-0.16837	-1.28626	1.84330
C	-1.32781	-1.99862	2.15395
C	-1.38617	-3.37280	1.92074
C	-0.28313	-4.02938	1.37369
C	0.87512	-3.31393	1.06260
H	1.72407	-3.84852	0.61056
H	-0.32922	-5.11378	1.17607
H	-2.30387	-3.93607	2.16043
H	-2.20130	-1.47141	2.57369
H	-0.14630	-0.20047	2.02267
C	3.09425	-0.63535	-5.16965
C	3.55371	-0.11906	-6.38261
C	4.76459	0.57315	-6.43356
C	5.51268	0.75192	-5.26864
C	5.05557	0.23071	-4.05636
H	5.64839	0.38987	-3.14042
H	6.46316	1.31080	-5.30424
H	5.12490	0.98705	-7.39056
H	2.95251	-0.24989	-7.29839
H	2.12369	-1.15662	-5.14372
C	0.86371	-2.51354	-2.32504
C	-0.01106	-3.56113	-2.61718
C	0.40508	-4.60723	-3.44283
C	1.69714	-4.60513	-3.97289
C	2.57576	-3.56222	-3.67163
H	3.59658	-3.57236	-4.08836
H	2.02648	-5.43101	-4.62592
H	-0.28645	-5.43447	-3.67620
H	-1.03012	-3.56057	-2.19520
H	0.52786	-1.68937	-1.67445
C	0.80711	4.83760	-4.98639
C	1.86048	5.56025	-5.54991
C	2.68675	4.96228	-6.50265
C	2.46189	3.63875	-6.88414
C	1.40840	2.91656	-6.31996
H	1.26690	1.86420	-6.61177
H	3.12575	3.15740	-7.62198
H	3.52419	5.52989	-6.94257
H	2.04641	6.60046	-5.23298
H	0.17578	5.31266	-4.21681
C	-1.29825	1.07202	-6.88755

C	-1.41490	-0.13506	-7.57984
C	-1.23175	-1.34572	-6.90944
C	-0.93462	-1.34752	-5.54578
C	-0.81866	-0.14080	-4.85352
H	-0.57763	-0.15101	-3.77826
H	-0.78769	-2.30292	-5.01625
H	-1.32111	-2.29989	-7.45585
H	-1.64836	-0.13168	-8.65805
H	-1.43373	2.02183	-7.43064
C	-2.72023	0.01272	-1.19008
C	-3.33161	-1.17369	-0.78193
C	-4.62944	-1.14864	-0.26865
C	-5.31406	0.06408	-0.16532
C	-4.70019	1.25170	-0.56979
H	-5.24560	2.20479	-0.47086
H	-6.33938	0.08500	0.24135
H	-5.11263	-2.08589	0.05554
H	-2.78603	-2.12907	-0.86047
H	-1.69446	-0.01672	-1.59193
C	-2.73150	3.26644	1.18183
C	-2.61869	4.08689	2.30634
C	-2.22165	5.41741	2.16582
C	-1.93229	5.92517	0.89866
C	-2.04787	5.10525	-0.22548
H	-3.00546	2.20856	1.32095
H	-2.82516	3.67690	3.30948
H	-2.12189	6.06177	3.05564
H	-1.59959	6.97100	0.78664
H	-1.78633	5.50959	-1.21770

Exo(B)

E: -1169,8855811

Pt	-1.79538	-0.26079	0.69661
Pt	1.40473	-0.75707	0.19645
S	-0.01500	1.25573	-0.13463
S	-0.03854	-1.11492	2.07563
C	-5.17511	0.55681	-0.05760
C	-5.58775	-0.87565	0.36482
C	-4.95971	-1.36920	1.69491
C	4.48497	-0.66915	-1.55479
C	4.81927	-2.09930	-1.05680
C	4.47992	-2.38649	0.42793
H	-5.87565	0.94914	-0.80062
H	-5.23545	1.21899	0.81439
H	-5.38951	-1.59181	-0.44491
H	-6.67574	-0.87293	0.49876
H	-5.52947	-2.22019	2.08351
H	-5.00735	-0.57643	2.45079
H	4.98576	-0.48628	-2.51109
H	4.85496	0.07510	-0.83974
H	4.35499	-2.84548	-1.71546
H	5.90109	-2.23651	-1.17068
H	4.99894	-3.29015	0.76659
H	4.84604	-1.56239	1.05409
C	0.47824	2.25975	1.26652
C	1.81659	2.62168	1.45922
C	2.16036	3.45264	2.52020
N	1.28857	3.94793	3.36804
C	0.02534	3.63503	3.19498
C	-0.43490	2.81048	2.17142
F	-1.75272	2.56611	2.07274
F	2.78347	2.17597	0.63289
F	3.44751	3.77366	2.69478
F	-0.86272	4.14657	4.05355
P	-3.42842	0.68608	-0.69648
P	-3.18052	-1.87519	1.51359
P	2.67122	-2.54510	0.84343
P	2.65350	-0.40709	-1.74878
C	-3.44486	-0.05110	-2.36916
C	-3.17309	2.45564	-1.07737
C	-2.63218	-2.54328	3.12436
C	-3.31022	-3.33702	0.42373
C	2.67986	-2.74253	2.66072
C	2.09182	-4.16299	0.22028
C	2.24314	-1.59253	-3.07842
C	2.39733	1.18964	-2.60107
C	-2.48477	2.85385	-2.22919

C	-2.26787	4.20799	-2.49160
C	-2.72990	5.17627	-1.59974
C	-3.40426	4.78626	-0.44227
C	-3.61982	3.43176	-0.18056
H	-2.09117	2.10735	-2.93703
H	-1.72134	4.51208	-3.40036
H	-2.55384	6.24599	-1.80395
H	-3.75826	5.54807	0.27289
H	-4.13196	3.14368	0.75147
C	-2.25642	-0.62742	-2.83038
C	-2.19246	-1.19338	-4.10448
C	-3.31756	-1.17910	-4.92963
C	-4.50057	-0.58865	-4.48139
C	-4.56207	-0.01919	-3.20738
H	-5.49814	0.45916	-2.87940
H	-5.38720	-0.56583	-5.13751
H	-3.26913	-1.62538	-5.93732
H	-1.25174	-1.64596	-4.46034
H	-1.35778	-0.63135	-2.19177
C	-1.99620	-3.78461	3.22979
C	-1.55533	-4.24670	4.47131
C	-1.74451	-3.46860	5.61438
C	-2.37289	-2.22626	5.51327
C	-2.81071	-1.76284	4.27087
H	-3.28175	-0.76834	4.19941
H	-2.51132	-1.60351	6.41330
H	-1.38769	-3.82960	6.59383
H	-1.04457	-5.22169	4.54601
H	-1.81692	-4.40310	2.33601
C	-2.54395	-3.36330	-0.74227
C	-2.63861	-4.44145	-1.62322
C	-3.48436	-5.51167	-1.32668
C	-4.23462	-5.49979	-0.14905
C	-4.15034	-4.41268	0.72370
H	-4.75217	-4.41091	1.64739
H	-4.90100	-6.34627	0.08853
H	-3.55803	-6.36583	-2.02089
H	-2.04297	-4.44730	-2.55113
H	-1.86297	-2.52929	-0.97073
C	2.99175	-1.61875	3.43384
C	3.00081	-1.70208	4.82742
C	2.70369	-2.91221	5.45615
C	2.40580	-4.03941	4.68873
C	2.39814	-3.95643	3.29466
H	2.16303	-4.85906	2.70875
H	2.17393	-4.99742	5.18429
H	2.70569	-2.97781	6.55737
H	3.23755	-0.80969	5.43125
H	3.22017	-0.65560	2.94647
C	2.94605	-5.10242	-0.36429
C	2.44525	-6.32358	-0.82084
C	1.08823	-6.61908	-0.68550
C	0.23242	-5.68863	-0.09608
C	0.73146	-4.46240	0.34561
H	0.04377	-3.73304	0.80116
H	-0.83848	-5.92241	0.02260
H	0.69373	-7.58641	-1.03978
H	3.12507	-7.05806	-1.28505
H	4.02180	-4.89630	-0.47360
C	1.29362	-2.58196	-2.81404
C	0.96370	-3.51842	-3.79474
C	1.56769	-3.45380	-5.05166
C	2.50408	-2.45419	-5.32417
C	2.84339	-1.52530	-4.33804
H	3.58504	-0.74066	-4.56177
H	2.98010	-2.40074	-6.31794
H	1.30627	-4.19253	-5.82816
H	0.22818	-4.30993	-3.57416
H	0.80458	-2.62981	-1.82794
C	1.26978	1.36185	-3.41128
C	1.04346	2.57914	-4.05578
C	1.93872	3.63604	-3.88528
C	3.05995	3.47216	-3.06998
C	3.28738	2.25287	-2.42813
H	0.54596	0.54095	-3.54265
H	0.15329	2.70626	-4.69486
H	1.75807	4.60039	-4.38967
H	3.76464	4.30889	-2.92722
H	4.16997	2.14382	-1.77751

TS endo-exo(A) ($\theta_1=180$)

E: -1169.87880594

Pt	-2.34105	0.02521	0.36702
Pt	1.26905	0.14411	0.43773
S	-0.51207	-1.07460	1.64416
S	-0.55394	1.14962	-0.73813
C	-5.84259	-0.86584	0.82254
C	-6.25159	0.48384	0.18800
C	-5.45832	0.88132	-1.08011
C	4.74374	-0.67613	0.96142
C	5.11467	0.73621	0.44864
C	4.41055	1.13451	-0.87055
H	-6.55930	-1.14658	1.60216
H	-5.89275	-1.65067	0.05629
H	-6.21137	1.29730	0.92327
H	-7.30709	0.39639	-0.09645
H	-5.98602	1.67986	-1.61364
H	-5.37660	0.03019	-1.76663
H	5.46933	-1.00562	1.71139
H	4.79794	-1.39037	0.13117
H	4.93982	1.49205	1.22714
H	6.19506	0.74513	0.26358
H	4.94577	1.95760	-1.35507
H	4.42761	0.29214	-1.57378
C	-0.42812	-2.79791	1.14545
C	-0.60171	-3.79893	2.11180
C	-0.51391	-5.13825	1.73676
N	-0.27326	-5.53326	0.50724
C	-0.11193	-4.60934	-0.41306
C	-0.18274	-3.24037	-0.16068
F	-0.01728	-2.37396	-1.16637
F	-0.84927	-3.48360	3.39344
F	-0.68021	-6.08189	2.66867
F	0.13166	-5.02023	-1.66208
P	-4.11420	-1.00772	1.53080
P	-3.74313	1.47452	-0.69473
P	2.62752	1.61308	-0.67052
P	3.02720	-0.78995	1.68360
C	-4.18712	-0.42795	3.26289
C	-4.03722	-2.82946	1.66088
C	-3.08639	2.19594	-2.24064
C	-4.05143	2.90257	0.40400
C	2.06117	1.93666	-2.37818
C	2.63973	3.24082	0.16129
C	3.20569	0.04106	3.30198
C	2.86496	-2.55303	2.13836
C	-4.41307	-3.53534	2.80659
C	-4.35029	-4.93038	2.82229
C	-3.94110	-5.62621	1.68346
C	-3.59604	-4.92551	0.52683
C	-3.64165	-3.53035	0.51700
H	-4.77166	-3.00484	3.70322
H	-4.63686	-5.48417	3.73228
H	-3.89818	-6.72843	1.69468
H	-3.28781	-5.47488	-0.37883
H	-3.37511	-2.98330	-0.40339
C	-3.18450	-0.81928	4.15628
C	-3.19468	-0.36985	5.47776
C	-4.20367	0.48862	5.91506
C	-5.19729	0.89840	5.02534
C	-5.18529	0.44586	3.70431
H	-5.96930	0.79766	3.01733
H	-5.98958	1.58772	5.36335
H	-4.21133	0.84822	6.95793
H	-2.40073	-0.68957	6.17383
H	-2.37509	-1.48774	3.82580
C	-2.54224	3.48373	-2.28359
C	-2.06079	4.00366	-3.48650
C	-2.11100	3.23537	-4.65056
C	-2.62843	1.93998	-4.60689
C	-3.11304	1.42134	-3.40458
H	-3.51145	0.39342	-3.38011
H	-2.65063	1.32378	-5.52164
H	-1.72785	3.64556	-5.60018
H	-1.63201	5.01972	-3.51409
H	-2.47588	4.09777	-1.37086

C	-3.42326	2.91712	1.65220
C	-3.63609	3.97949	2.53207
C	-4.47433	5.03340	2.16316
C	-5.09986	5.02259	0.91452
C	-4.89017	3.95752	0.03587
H	-5.38903	3.95709	-0.94741
H	-5.76203	5.85524	0.62245
H	-4.64310	5.87333	2.85821
H	-3.14385	3.98238	3.51932
H	-2.76176	2.08691	1.95099
C	1.89638	0.83287	-3.22165
C	1.47694	1.01058	-4.54116
C	1.22750	2.29489	-5.02665
C	1.38703	3.39869	-4.18714
C	1.79820	3.22024	-2.86456
H	1.90667	4.10326	-2.21536
H	1.18147	4.41384	-4.56698
H	0.89700	2.43617	-6.06960
H	1.34148	0.13529	-5.19875
H	2.08914	-0.18633	-2.84591
C	3.61848	4.20608	-0.09418
C	3.58081	5.43755	0.56362
C	2.56122	5.71330	1.47624
C	1.57691	4.75645	1.72750
C	1.61624	3.52591	1.06990
H	0.83036	2.78136	1.27366
H	0.76604	4.97187	2.44387
H	2.53138	6.68638	1.99510
H	4.35676	6.19481	0.35956
H	4.42430	4.01129	-0.81960
C	2.24476	0.99105	3.65666
C	2.33001	1.65588	4.88095
C	3.37492	1.36654	5.76024
C	4.33112	0.40982	5.41396
C	4.24598	-0.25344	4.18785
H	5.00157	-1.01420	3.93242
H	5.15412	0.17619	6.11053
H	3.44342	1.89128	6.72822
H	1.57091	2.40896	5.15226
H	1.41282	1.21880	2.97115
C	2.47864	-2.95659	3.42039
C	2.37665	-4.31441	3.73035
C	2.64413	-5.27703	2.75603
C	2.99850	-4.87931	1.46631
C	3.10203	-3.52176	1.15741
H	2.24149	-2.21328	4.19838
H	2.07333	-4.62638	4.74403
H	2.55745	-6.34943	2.99953
H	3.18995	-5.63835	0.68903
H	3.36893	-3.22268	0.13032

TS exo(A)-exo(B) ($\theta_2=20$)

E: -1169,87926596

Pt	-1.78610	-0.47617	0.73129
Pt	1.53594	-0.88370	0.25192
S	0.00731	1.04971	0.00334
S	-0.04243	-1.64894	1.87200
C	-5.14130	0.65874	0.31969
C	-5.61467	-0.81251	0.43735
C	-4.98320	-1.61282	1.60742
C	4.72629	-0.73717	-1.36839
C	4.93709	-2.24380	-1.07497
C	4.52372	-2.70357	0.34607
H	-5.83618	1.22852	-0.30384
H	-5.15591	1.12555	1.31241
H	-5.47194	-1.34285	-0.51473
H	-6.69784	-0.79115	0.60466
H	-5.58806	-2.50131	1.81906
H	-4.97339	-1.00291	2.51846
H	5.26170	-0.46136	-2.28247
H	5.14719	-0.14000	-0.55051
H	4.43988	-2.85243	-1.84237
H	6.00881	-2.44773	-1.18368
H	4.98607	-3.66775	0.58390
H	4.89364	-1.98697	1.09106

C	0.32791	2.29147	1.26073
C	0.93078	3.48387	0.83089
C	1.16613	4.51150	1.73776
N	0.85236	4.43843	3.01117
C	0.28228	3.33433	3.43384
C	-0.00179	2.23539	2.62154
F	-0.62240	1.18404	3.16343
F	1.27262	3.65058	-0.45731
F	1.73697	5.63934	1.30233
F	-0.05183	3.26956	4.72711
P	-3.40047	0.85180	-0.31850
P	-3.23845	-2.15151	1.25965
P	2.69058	-2.82232	0.63821
P	2.92967	-0.26915	-1.53753
C	-3.47213	0.66751	-2.13577
C	-2.99840	2.62019	-0.08884
C	-2.67918	-3.18436	2.66038
C	-3.47706	-3.33559	-0.11243
C	2.55418	-3.37750	2.37451
C	2.08093	-4.24479	-0.33467
C	2.42123	-1.18776	-3.03394
C	2.90141	1.44274	-2.17803
C	-2.57658	3.44078	-1.13960
C	-2.23100	4.77211	-0.89739
C	-2.29871	5.28985	0.39696
C	-2.70975	4.47272	1.45075
C	-3.05125	3.14069	1.20894
H	-2.48879	3.04655	-2.16449
H	-1.89046	5.41183	-1.72911
H	-2.01836	6.33955	0.58800
H	-2.75218	4.87573	2.47688
H	-3.34426	2.49702	2.05517
C	-2.34993	0.13976	-2.78321
C	-2.33892	-0.01351	-4.17026
C	-3.45040	0.37059	-4.92146
C	-4.56632	0.91464	-4.28276
C	-4.57511	1.06848	-2.89441
H	-5.45731	1.51684	-2.41111
H	-5.44126	1.22913	-4.87666
H	-3.44386	0.25187	-6.01819
H	-1.44987	-0.43326	-4.67099
H	-1.46090	-0.15589	-2.20377
C	-2.05032	-4.41685	2.45376
C	-1.60501	-5.17085	3.54099
C	-1.77500	-4.69172	4.84072
C	-2.38917	-3.45601	5.05104
C	-2.83573	-2.70243	3.96348
H	-3.29567	-1.71621	4.14106
H	-2.50956	-3.06766	6.07656
H	-1.41198	-5.28187	5.69914
H	-1.10400	-6.13879	3.37062
H	-1.88010	-4.79823	1.43402
C	-2.80657	-3.10251	-1.31427
C	-2.98317	-3.96490	-2.39728
C	-3.81739	-5.07740	-2.27349
C	-4.47744	-5.32188	-1.06744
C	-4.31116	-4.44987	0.01070
H	-4.84226	-4.64789	0.95646
H	-5.13699	-6.20061	-0.96817
H	-3.95622	-5.76122	-3.12796
H	-2.46376	-3.76634	-3.34967
H	-2.13867	-2.23285	-1.41132
C	2.88430	-2.46278	3.38012
C	2.78847	-2.82793	4.72427
C	2.36809	-4.11303	5.07033
C	2.04879	-5.03261	4.07011
C	2.14242	-4.66678	2.72557
H	1.88131	-5.40677	1.95246
H	1.71699	-6.04894	4.34222
H	2.28719	-4.40077	6.13224
H	3.03929	-2.09817	5.51263
H	3.20926	-1.44197	3.11676
C	2.93912	-5.20486	-0.88025
C	2.42546	-6.28080	-1.60752
C	1.04780	-6.41366	-1.78357
C	0.18522	-5.46768	-1.23024
C	0.70065	-4.38710	-0.51285
H	0.00512	-3.64898	-0.08512
H	-0.90462	-5.57573	-1.35645
H	0.64156	-7.26647	-2.35329

H	3.11029	-7.03045	-2.03901
H	4.02895	-5.13078	-0.74369
C	1.26543	-1.96862	-2.95989
C	0.83324	-2.69166	-4.07239
C	1.54720	-2.62102	-5.26982
C	2.69159	-1.82493	-5.35251
C	3.12746	-1.10714	-4.23655
H	4.02687	-0.47462	-4.31538
H	3.25248	-1.76278	-6.30046
H	1.20665	-3.19228	-6.14999
H	-0.07022	-3.32007	-4.00291
H	0.69103	-2.01758	-2.02073
C	1.87799	1.84421	-3.04405
C	1.85241	3.14556	-3.54926
C	2.84498	4.05640	-3.18370
C	3.85562	3.66671	-2.30290
C	3.88005	2.36520	-1.79653
H	1.07965	1.14061	-3.33299
H	1.04249	3.45550	-4.23115
H	2.82221	5.08644	-3.57794
H	4.63109	4.39053	-1.99988
H	4.67749	2.07763	-1.09252

II) Experimental details

a) Characterization of II

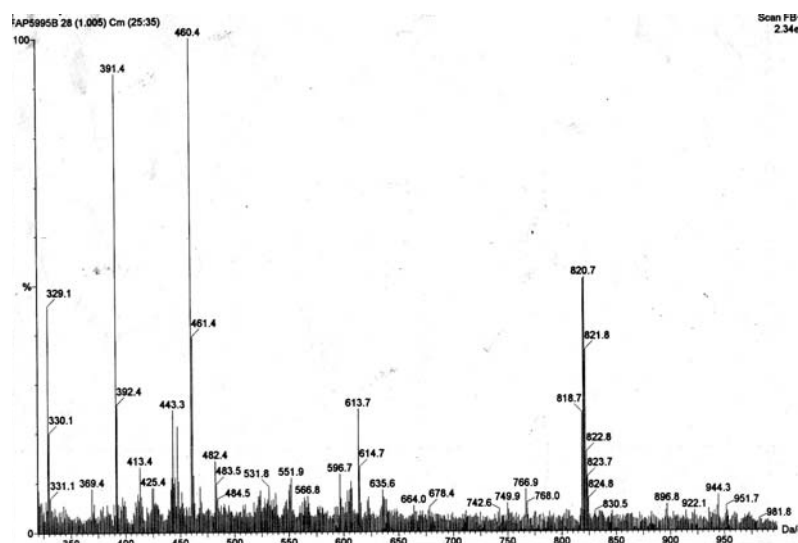


Figure S1 - FAB⁺ spectrum of II.

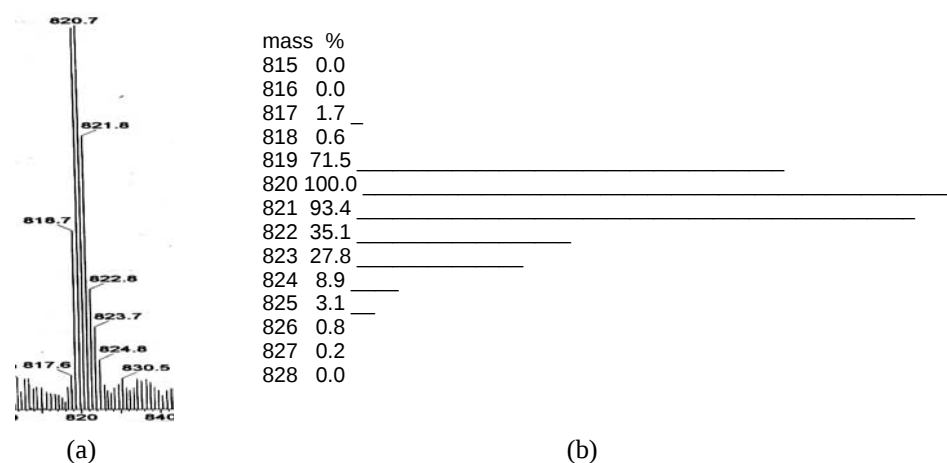


Figure S2 - (a) Region of the FAB⁺ spectrum corresponding to [Pt(dppp)(o-S₂C₆F₄)]H⁺ cation. (b) Simulation of the isotopic distribution for the [Pt(dppp)(o-S₂C₆F₄)]H⁺ cation.

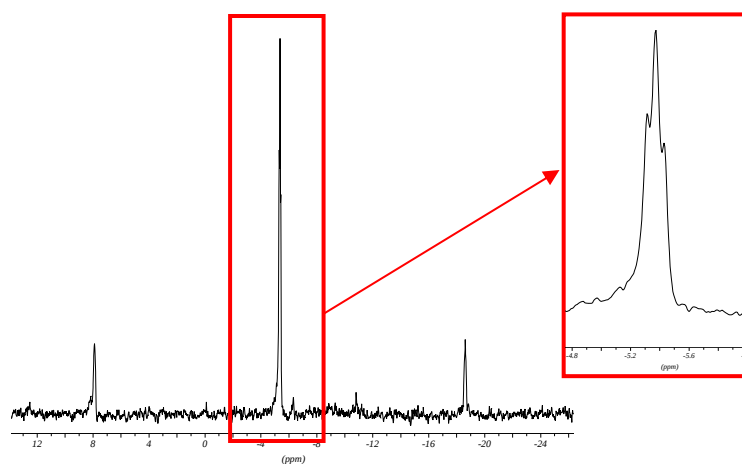


Figure S3. ³¹P{¹H} NMR spectrum obtained for [Pt(dppp)(o-S₂C₆F₄)] at room temperature, with the central signal enlargement

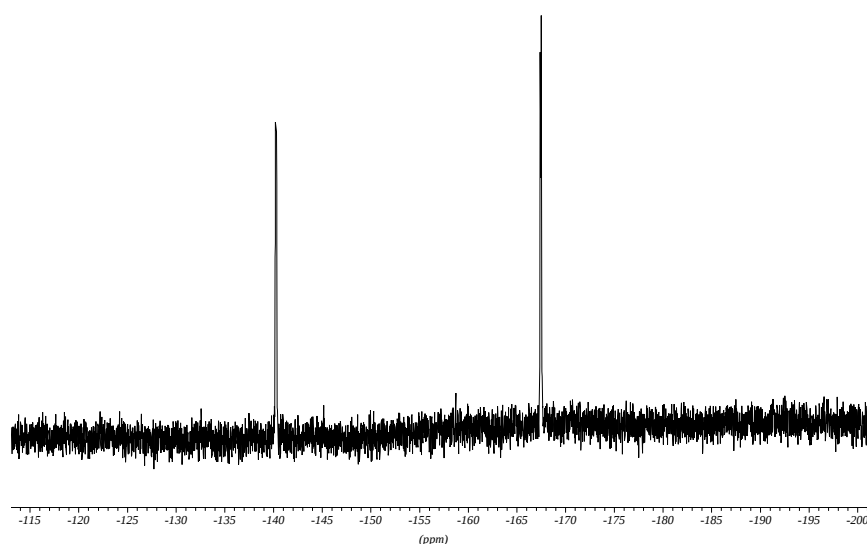


Figure S4. ^{19}F NMR spectrum obtained for product **II** at room temperature.

b) Characterization of **IV**

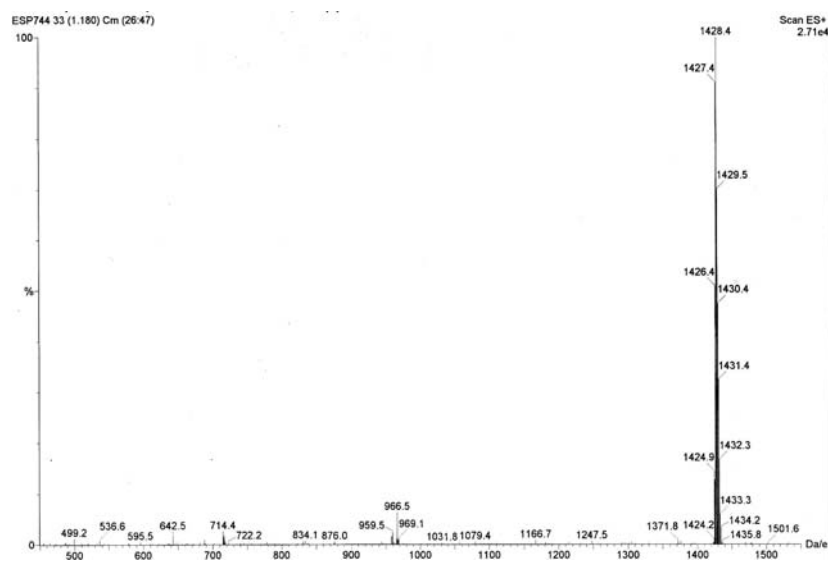
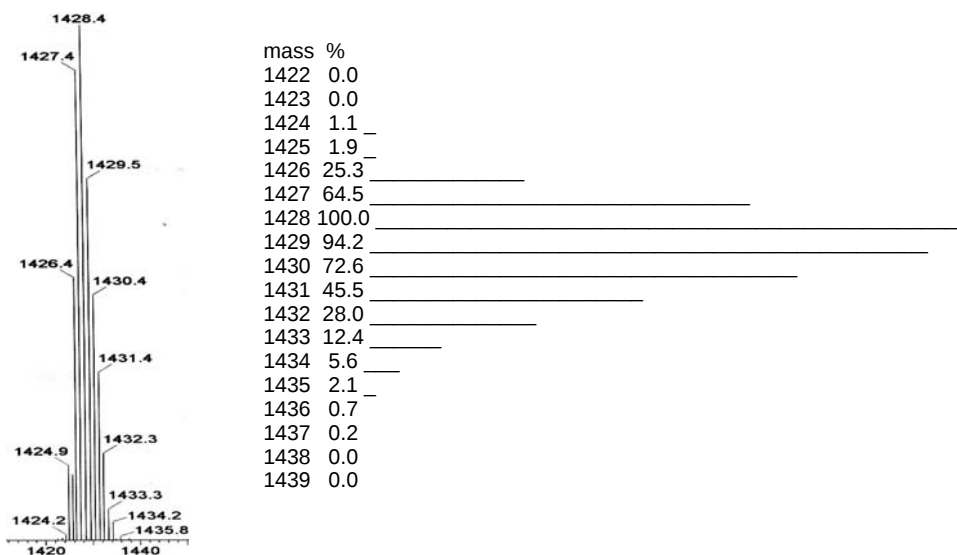


Figure S5 - ESI^+ spectrum of **IV**.



(a)

(b)

Figure S6 - (a) Region of the ESI⁺ spectrum corresponding to [Pt₂(dppp)₂(μ-S){μ-(*p*-SC₅F₄N)}]⁺ cation. (b) Simulation of the isotopic distribution for the [Pt₂(dppp)₂(μ-S){μ-(*p*-SC₅F₄N)}]⁺ cation.

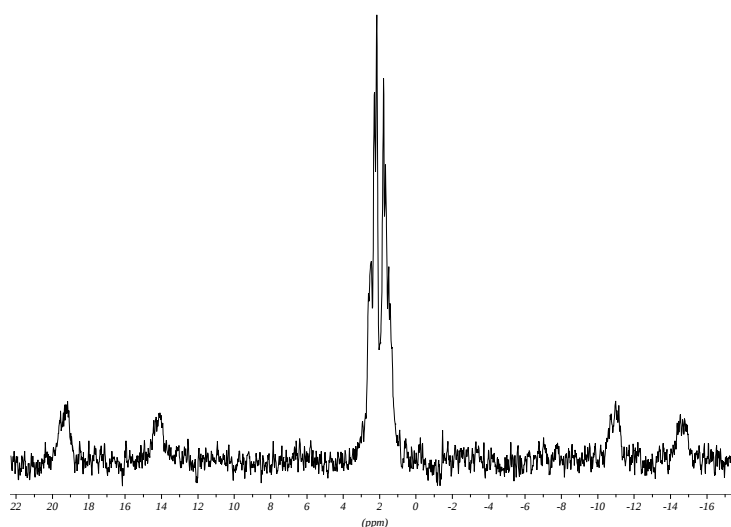


Figure S7. ³¹P{¹H}NMR spectrum obtained for product **IV** at room temperature.

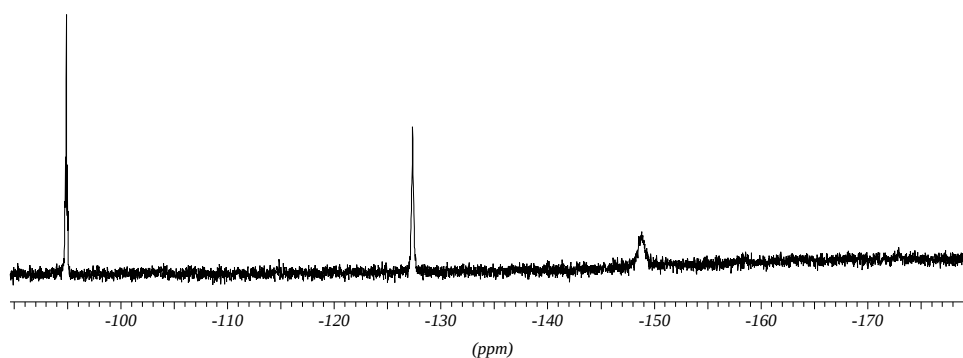


Figure S8. ¹⁹F NMR spectrum obtained for product **IV** at room temperature.

