Supporting Information (SI)

Ferrocene-Based Small Molecules for Dual Channel Sensing of Heavy and Transition Metal Cations

Antonio Caballero, Arturo Espinosa, Alberto Tárraga, * and Pedro Molina *

Departamento de Química Orgánica. Facultad de Química. Universidad de Murcia. Campus de Espinardo, E-30100 Murcia, Spain.

*E-mail: **pmolina@um.es**; atarraga@um.es*

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General Comments.-

Melting points were determined on a hot-plate melting point apparatus and are uncorrected. ^{1}H- and ^{13}C-NMR spectra were recorded at 400 and 100 MHz, respectively. The following abbreviations for stating the multiplicity of the signals have been used; s (singlet), d (doublet), st (pseudotriplet), m (multiplet), q (quaternary carbon). Chemical shifts refer to signals of tetramethylsilane in the case of ^{1}H and ^{13}C spectra. The FAB^{+} mass spectra were recorded using 3-nitrobenzylalcohol as a matrix. Electrochemical experiments were conducted in a conventional three-electrode cell under a nitrogen atmosphere at 25 ^{o}C. The working electrode was a Pt disk (1.6 mm in diameter) polished before each recording for cyclic and OSWV voltamperometric measurements and a platinum mesh for spectroelectrochemical experiments. The auxiliary electrode was a platinum wire. The reference electrode was SCE and decamethylferrocene (DMFc, -0.07 V *vs* SCE) was used as an internal reference both for potential calibration and for reversibility criteria. The experiments were carried out in acetonitrile solutions containing 0.1 M [(*n*-Bu)$_4$N]ClO$_4$ or 0.15 M [(*n*-Bu)$_4$N]PF$_6$ as supporting electrolyte. Deoxygenation of the solutions was achieved by bubbling nitrogen for at least 10 min and the working electrode was cleaned after each run. UV/Vis spectra were recorded before and after addition of sequential additions of aliquot of 0.1 equiv of 2.5x 10^{-2} M solutions of all the cation metal tested to a free ligand solutions (c = 1 x 10^{-4} M in CH_3CN).

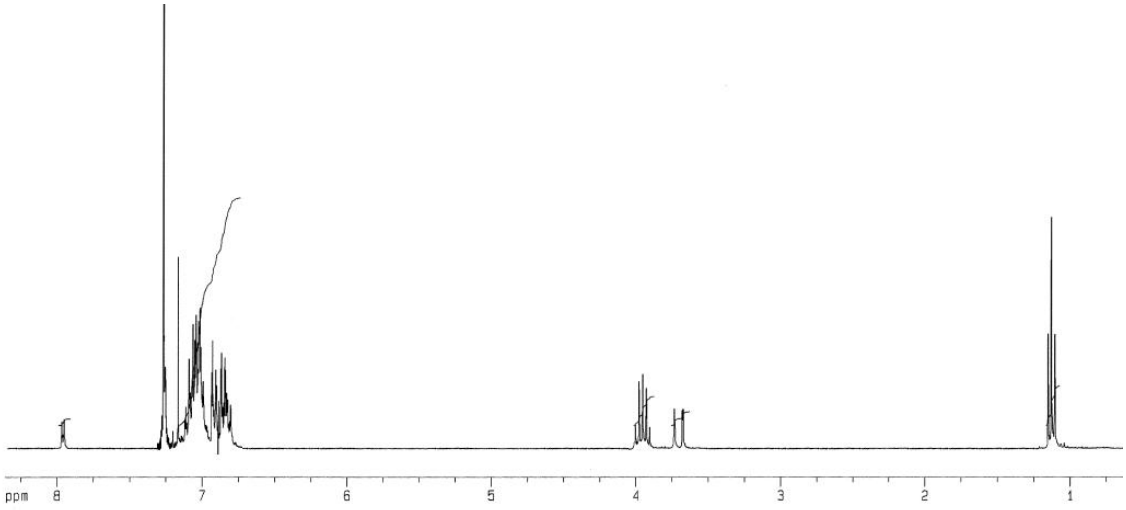
Computational details.-

Calculated geometries were fully optimized in the gas-phase with tight convergence criteria at the DFT level with the Gaussian 03 package,[1] using the B3LYP[2] functional and the 6-31G* basis set for all atoms excepting Pb and Hg for which the SDD basis set, with effective core potential (ecp), was employed. From these gas-phase optimized geometries all reported data were obtained by means of single-point (SP) calculations. The larger basis set 6-311G**, together with SDD-ecp (for Pb and Hg) was used to perform the Natural Bond Orbital (NBO) population analysis, from which natural charges were obtained. Bond orders were characterized by the Wiberg's bond index[3] (WBI) and calculated with the NBO method as the sum of squares of the off-diagonal density matrix elements between atoms. Energy values were computed at the B3LYP/6-

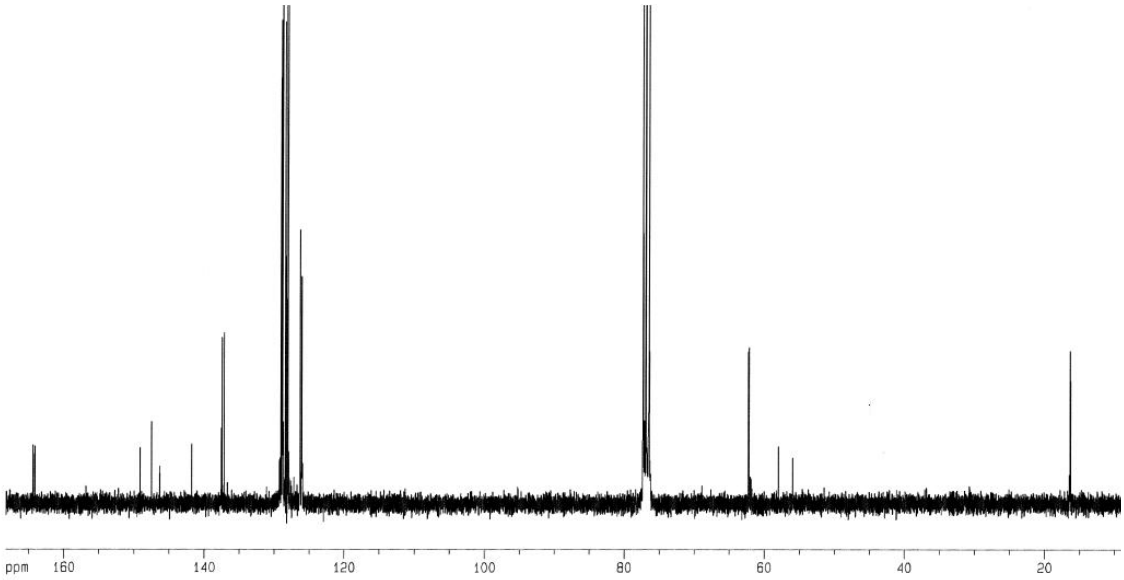
311G**/SDD-ecp level and considering solvent (acetonitrile or THF) effects by using the Cossi and Barone's CPCM (conductor-like conductor-like polarizable continuum model) modification[4] of the Tomasi's PCM (polarizable continuum model) formalism[5] and are uncorrected for the zero-point vibrational energy. Ligand strain energies (L_{strain}) were computed as the difference between the Gibbs free energy (in solution) of the free ligand in its most stable conformation and that of the frozen conformation of the ligand as obtained from the complex after removing the guest atoms and restoring the initial distances (as in the free ligand) to the bonds of atoms involved in guest binding (typically acidic C-H bonds).

Diethyl *N*-(pentakisphenylthio)bencylidenaminomethylphosphonate, 3.

^{1}H NMR (400 MHz, $CDCl_3$)

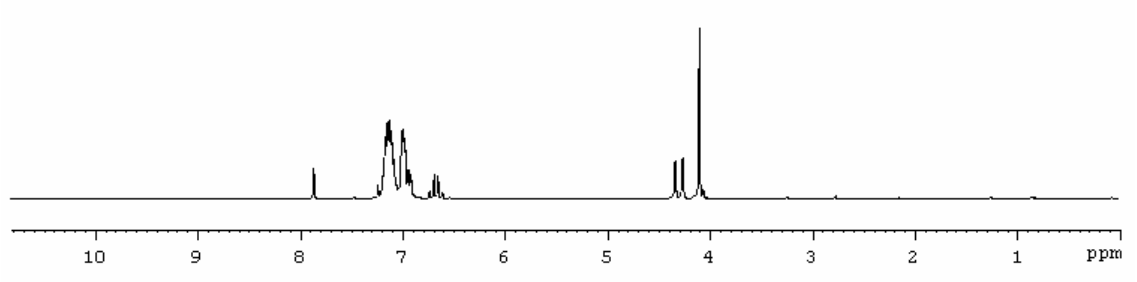


^{13}C NMR (100 MHz, $CDCl_3$)

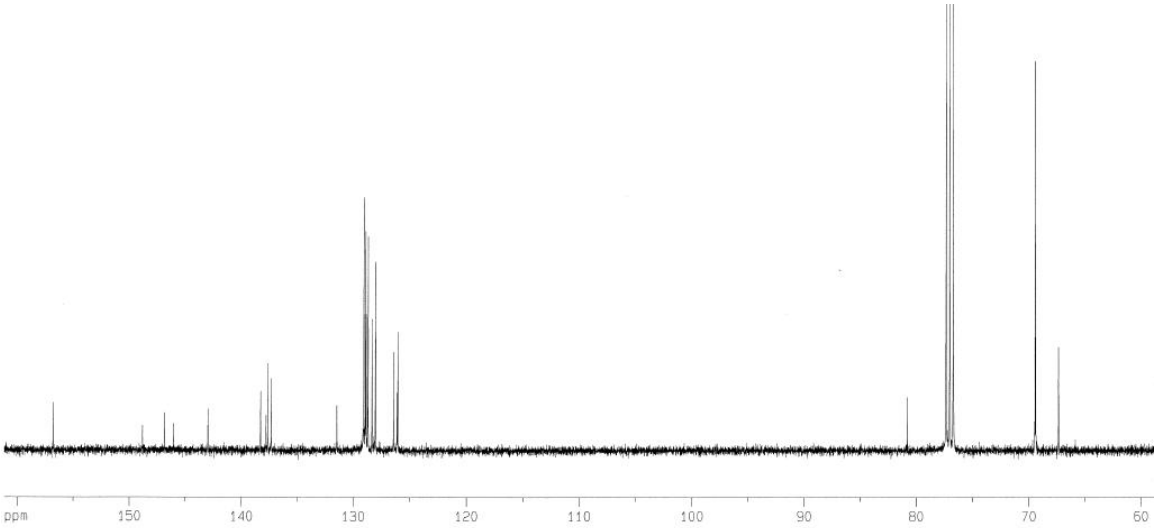


2-Aza-4-ferrocenyl-1-[pentakis(phenylthio)phenyl]-1,3-butadiene 5.

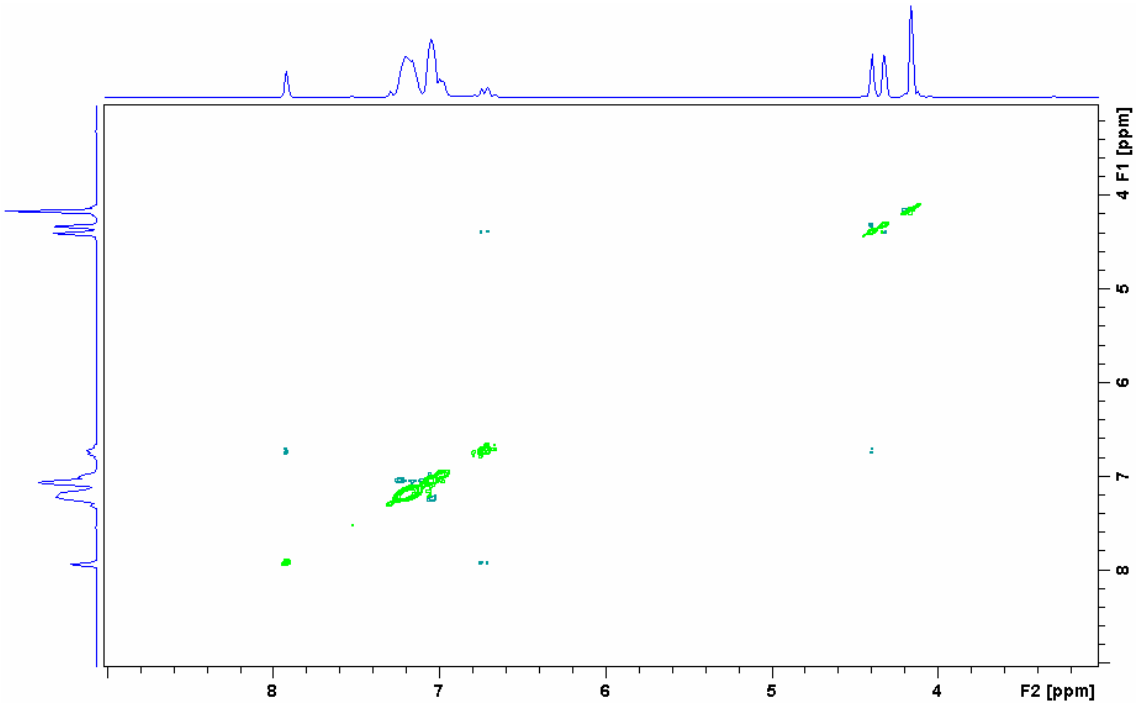
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)

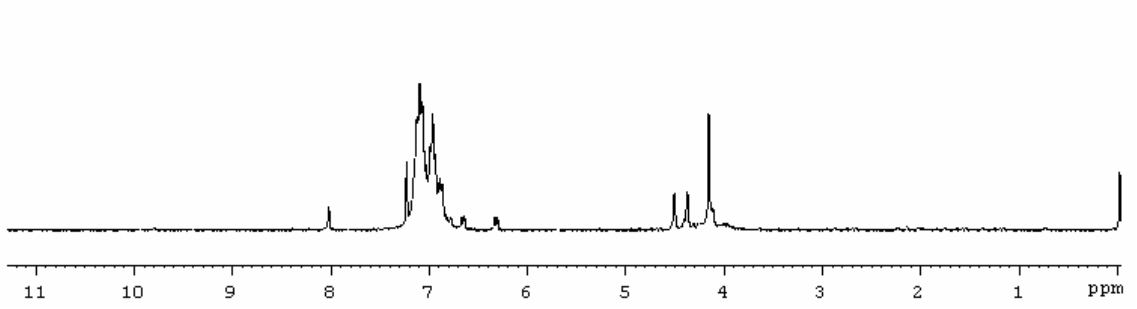


NOESY (400 MHz, $CDCl_3$)

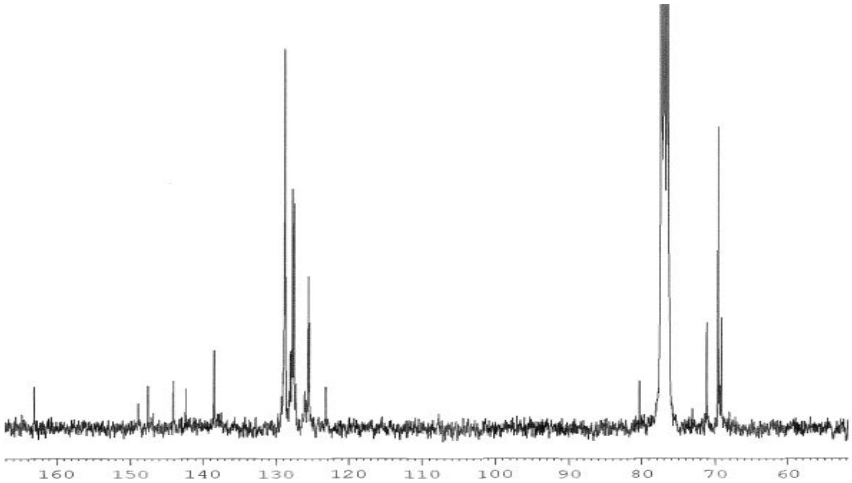


2-Aza-1-ferrocenyl-4-[pentakis(phenylthio)phenyl]-1,3-butadiene 7.

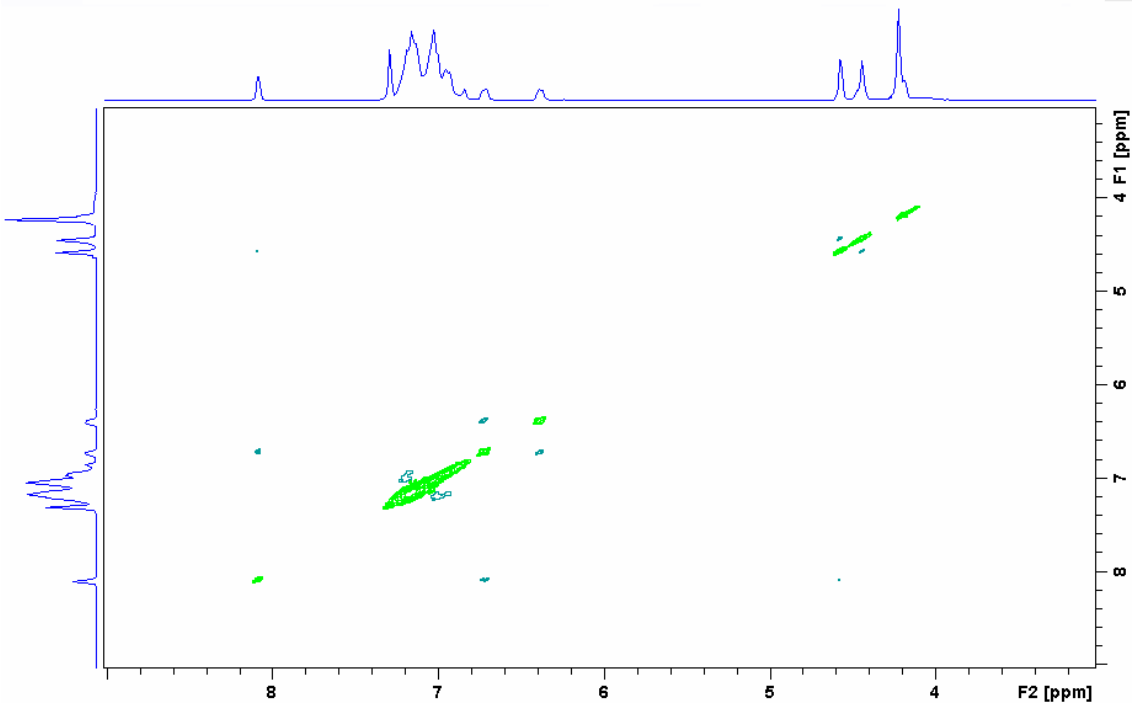
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



NOESY (400 MHz, $CDCl_3$)



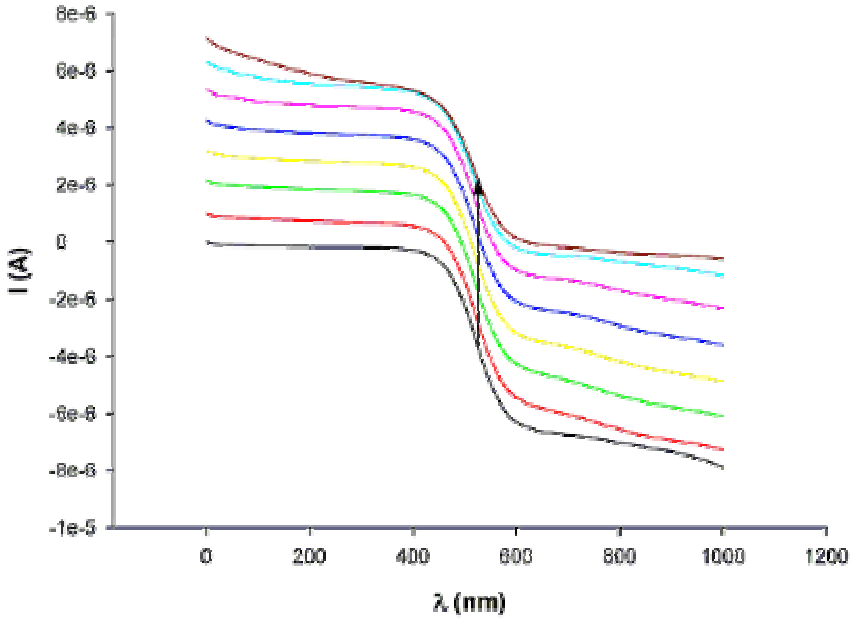


Figure SI 1. Changes in the linear sweep voltammogram of **5** (1 x 10^{-3} M) in CH_3CN with TBAP (0.1 M) as supporting electrolyte, obtained using a rotating disk electrode at 100 mV s^{-1} and 1000 rpm, upon addition of increasing amounts of Cu^{2+} cations.

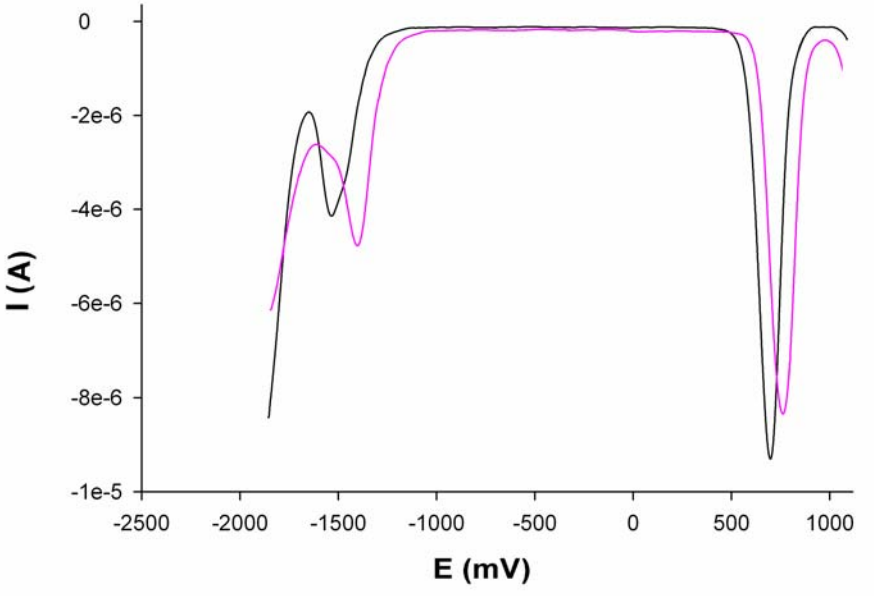


Figure SI 2. Changes of the OSWV of **5** (black) (1 mM, in MeOH/TBAP) scanned at 0.1 V s^{-1} in the presence of 1 equivalent of Pb^{2+} cations (pink).

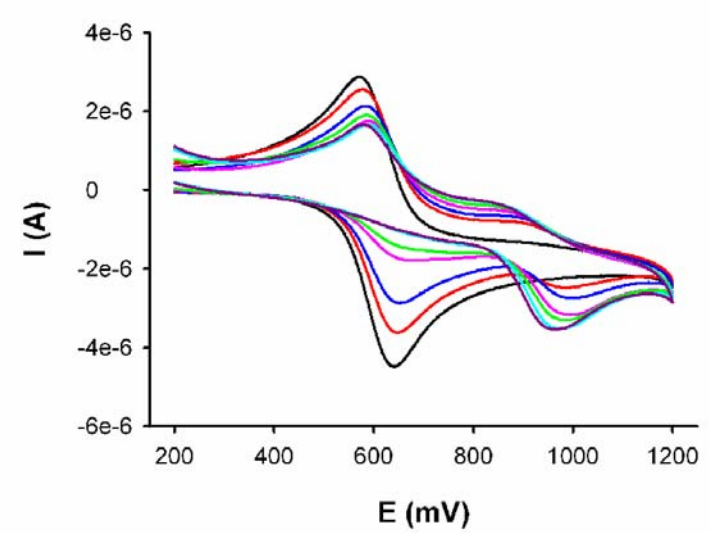


Figure SI 3. Evolution of the CV of **7** (black) (1 mM, in CH_3CN/TBAP) scanned at 0.1 V s^{-1} in the presence of increasing amounts of Hg^{2+}: the initial (black) is that of **7** and the final one (deep green), after addition of 1 equivalent of Hg^{2+} cations.

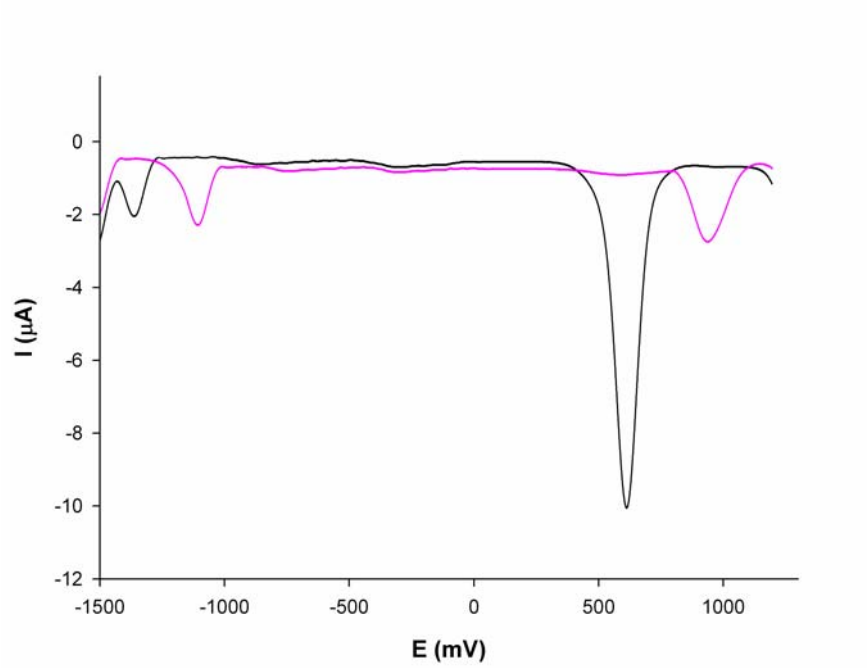


Figure SI 4. Changes of the OSWV of **7** (black) (1 mM, in MeOH/TBAP) scanned at 0.1 V s^{-1} in the presence of 1 equivalent of Hg^{2+} cations (pink).

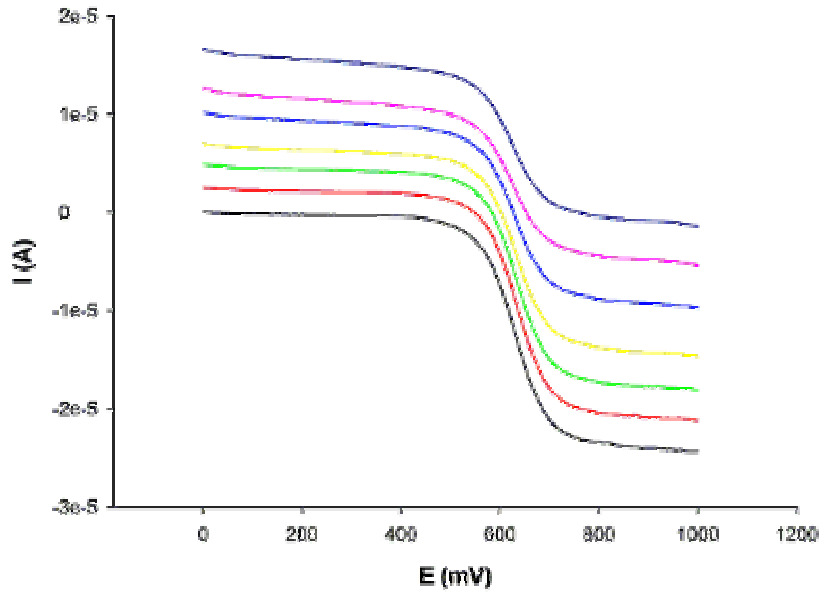


Figure SI 5. Changes in the linear sweep voltammogram of **7** (1 x 10^{-3} M) in CH_3CN with TBAP (0.1 M) as supporting electrolyte, obtained using a rotating disk electrode at 100 mV s^{-1} and 1000 rpm, upon addition of increasing amounts of Cu^{2+} cations

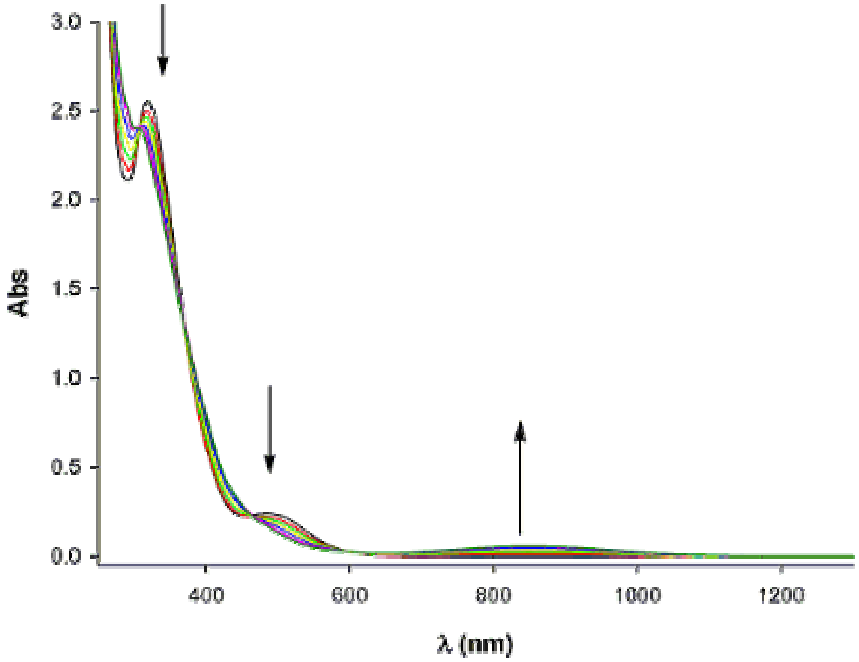


Figure SI 6. Changes in the absorption spectrum of **5** (1 x 10^{-4} M, in CH_3CN) upon addition of increasing amounts of Cu^{2+}.

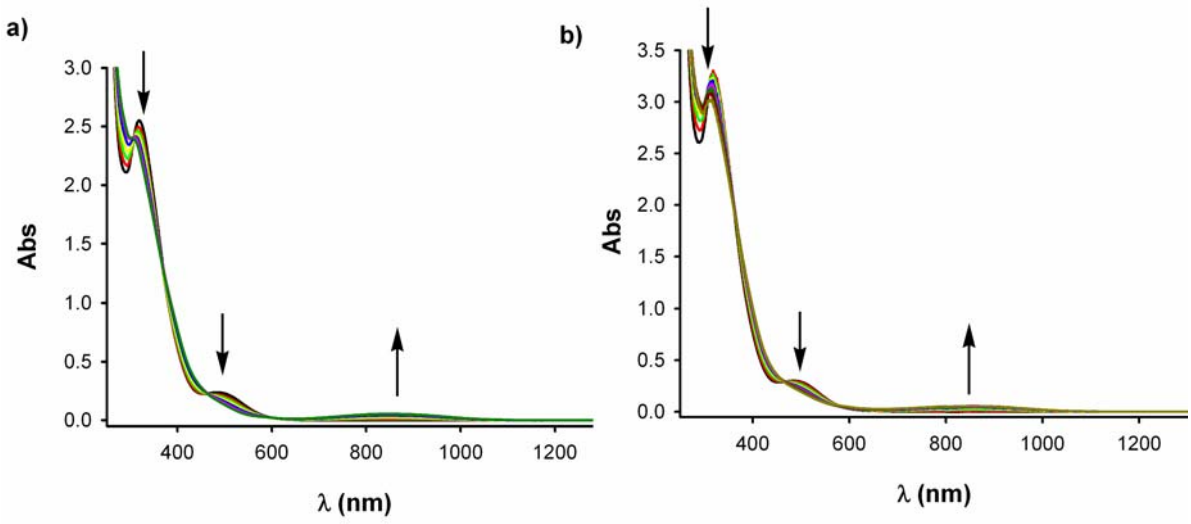


Figure SI 7. Changes in the UV-Vis-NIR spectrum of **5** (1 x 10^{-4} M, in CH_3CN); (a) upon addition of increasing amounts of Hg^{2+} and (b) evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **5** (1 x 10^{-4} M, in CH_3CN) with TBAP (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electron is removed. Arrows indicate absorptions that increase or decrease during the experiment.

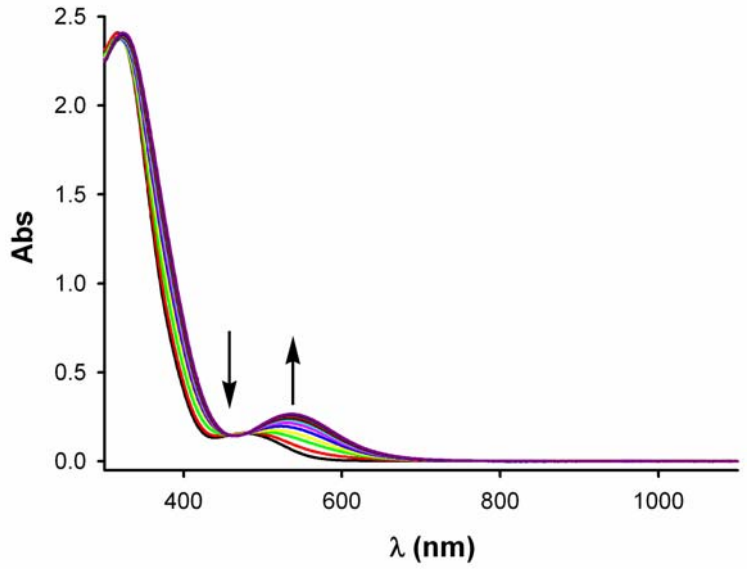


Figure SI 8. Changes in the absorption spectra of **7** (1 x 10^{-4} M) in CH_3CN upon addition of increasing amounts of Pb^{2+} (2.5 x 10^{-2} M) in CH_3CN. Arrows indicate absorptions that increase or decrease during the experiment.

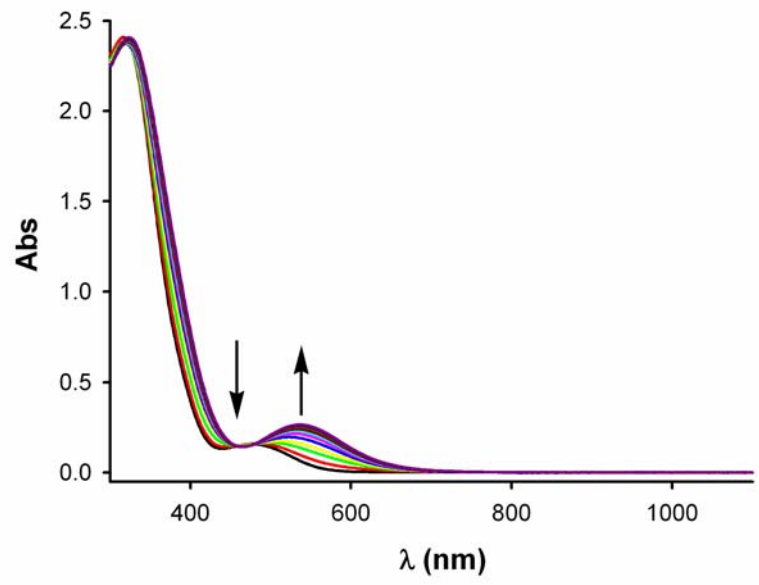


Figure SI 9. Changes in the absorption spectra of **7** (1 x 10^{-4} M) in CH_3CN upon addition of increasing amounts of Hg^{2+} (2.5 x 10^{-2} M) in CH_3CN. Arrows indicate absorptions that increase or decrease during the experiment.

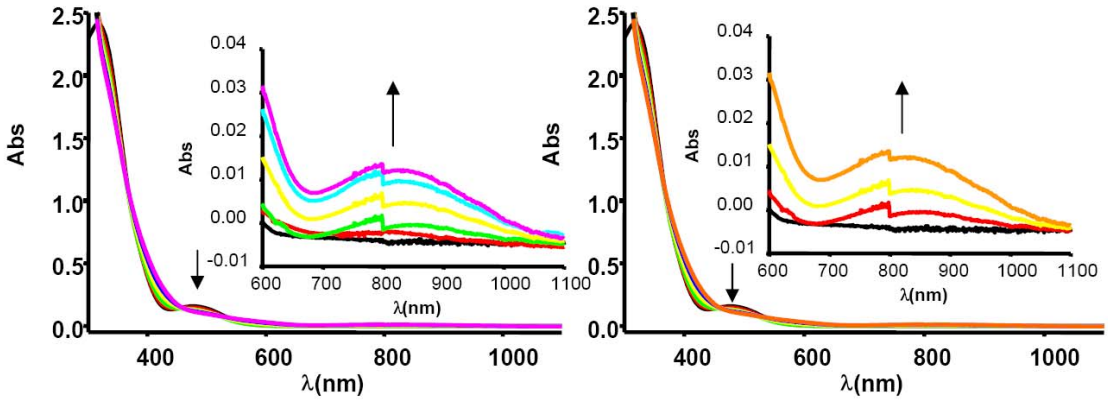


Figure SI 10. Changes in the UV-Vis-NIR spectrum of **7** (1 x 10^{-4} M, in CH_3CN); (a) upon addition of increasing amounts of Cu^{2+} and (b) evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **7** (1 x 10^{-4} M, in CH_3CN) with TBAP (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electron is removed. Arrows indicate absorptions that increase or decrease during the experiment.

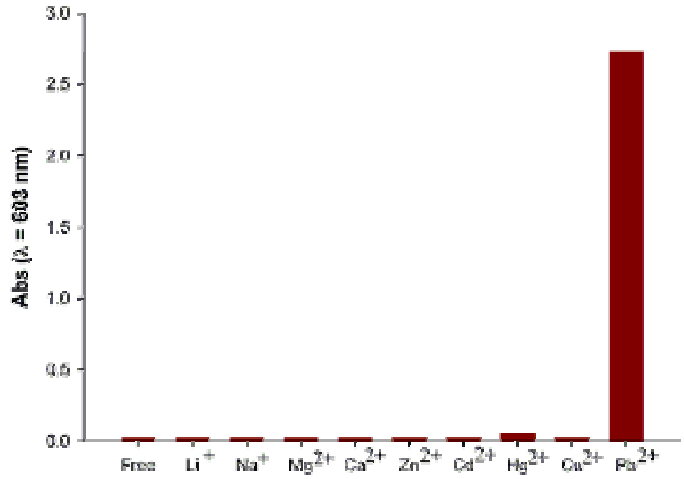


Figure SI 11. Absorption of ligand **5** (1 x 10^{-4} M, in CH_3CN) at λ = 603 nm after addition of several metal ions.

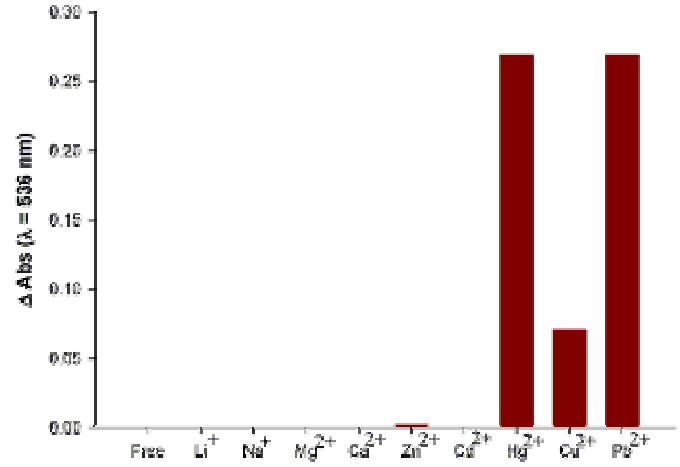


Figure SI 12. Absorption increase of ligand **7** (1 x 10^{-4} M, in CH_3CN) at λ = 536 nm, in relation to the free ligand, after addition of several cations.

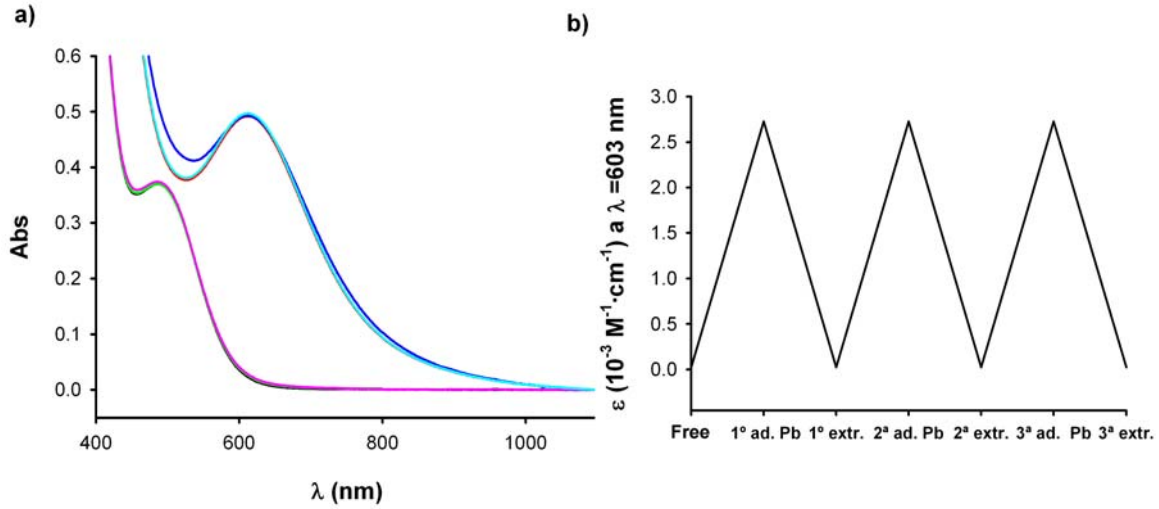


Figure SI 13. Stepwise complexation/decomplexation cycles, after addition of 1 equiv of Pb^{2+} cations and after extraction with water and recovery of the free receptor **5**. This reversible cycle can be repeated without loss of sensitivity.

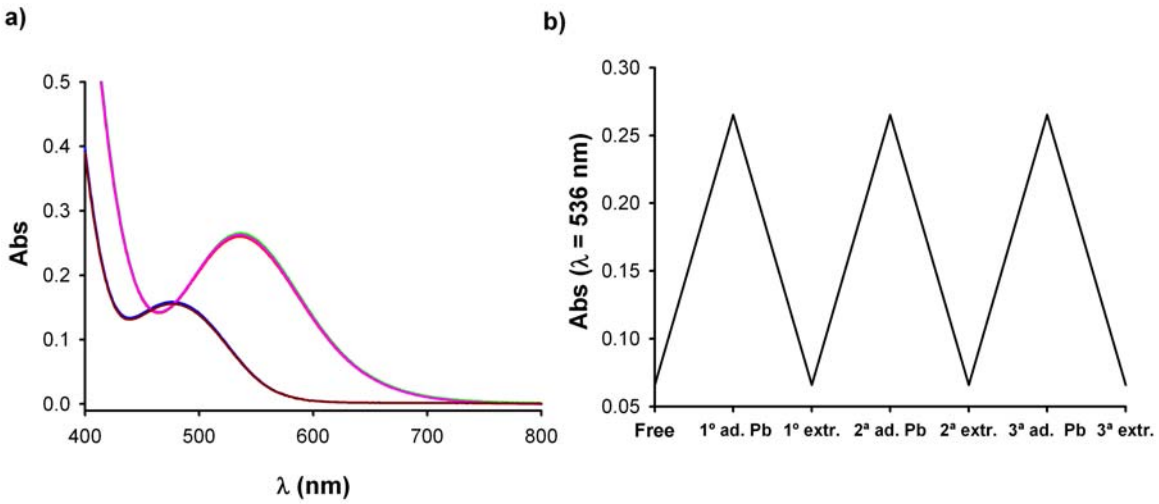


Figure SI 14. Stepwise complexation/decomplexation cycles, after addition of 1 equiv of Pb^{2+} cations and after extraction with water and recovery of the free receptor **7**. This reversible cycle can be repeated without loss of sensitivity.

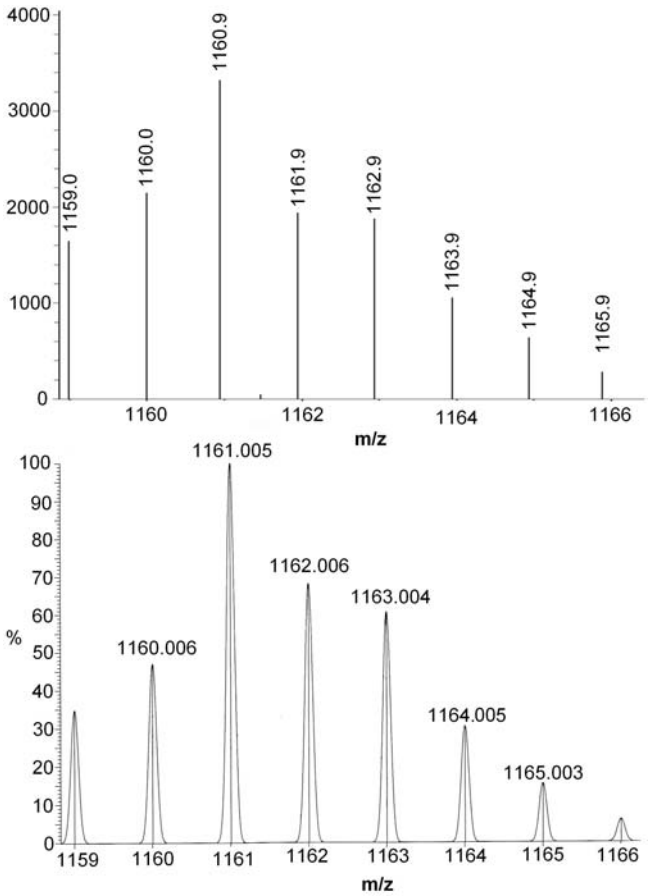


Figure SI 15. Electrospray mass spectrum of a $[\mathbf{5}\cdot Pb\cdot(ClO_4)]^+$ sample, in CH_3CN solution. Top: the measured pattern of the complex. Bottom: the calculated pattern of the complex.

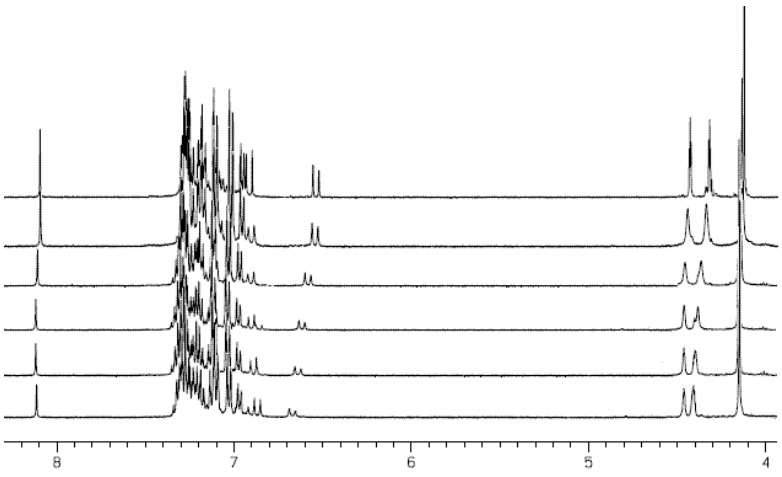


Figure SI 16. Evolution of the ^{1}H-NMR spectrum of **5** in CD_3CN (top) upon addition of increasing amounts of Pb^{2+} until 1 equivalents was added (botton).

Calculated structures: cartesian coordinates (in Å) and energies computed for FcH, $FcH^+ClO_4^-$, HPTB and derived complexes**.-**

FcH (D_{5h}): G_{MeCN} = -1650.886134 au

Fe	0.00000000	0.00000000	0.00000000
C	2.05213856	0.00000000	0.00000000
C	1.55538765	1.33867217	0.00000000
C	0.75162776	1.51104833	1.16750195
C	0.75162776	0.27891206	1.88905689
C	1.55538765	-0.65496816	1.16750156
H	2.68539081	-0.44356182	-0.75743174
H	1.74600263	2.08795278	-0.75743099
H	0.22604117	2.41392848	1.45038925
H	0.22604117	0.08387821	2.81489683
H	1.74600263	-1.68214780	1.45038867
C	-0.61432919	-0.98946576	-1.68962416
C	-1.11108010	0.34920641	-1.68962416
C	-1.91483999	0.52158257	-0.52212221
C	-1.91483999	-0.71055370	0.19943273
C	-1.11108010	-1.64443392	-0.52212260
H	0.03359921	-1.42758160	-2.43775627
H	-0.90578897	1.10393300	-2.43775553
H	-2.42575043	1.42990871	-0.22993528
H	-2.42575043	-0.90014157	1.13457230
H	-0.90578897	-2.66616758	-0.22993586

$FcH^+ClO_4^-$ (quasi-C_s): G_{MeCN} = -2411.697061 au

C	0.00000000	0.00000000	0.00000000
C	1.42999986	0.00000000	0.00000000
C	1.87380424	1.36058097	0.00000000
C	0.71179246	2.19727509	0.00096386
C	-0.44460169	1.35707424	0.00021709
H	-0.67232804	-0.84660265	-0.05768983
H	2.06827405	-0.87352665	-0.02952859
H	2.90246328	1.69604568	-0.02271229
H	0.71150186	3.27905873	-0.03207458
H	-1.48268305	1.65767261	-0.09182634
Fe	0.71770240	0.98547953	-1.67135313
C	-0.06786676	0.00207816	-3.31314811
C	-0.51206953	1.35914019	-3.29345643
C	0.64334559	2.19937102	-3.34050442
C	1.80440060	1.36270619	-3.38817604
C	1.36093355	0.00211490	-3.37170796
H	-0.73729012	-0.84461343	-3.22903586
H	-1.54550313	1.65959624	-3.15860293
H	0.64443597	3.28111237	-3.30612530
H	2.83313546	1.69816858	-3.40718671
H	1.99985912	-0.87143170	-3.36943747
Cl	-3.55492547	0.01109936	-1.58444349
O	-2.94313515	-0.63570569	-0.37295030
O	-2.99327675	-0.63417029	-2.82078394
O	-5.02708661	-0.11690712	-1.55436793
O	-3.16156306	1.47472640	-1.59158310

HPTB (quasi-S_6): G_{MeCN} = -4008.13024 au

C	0.00000000	0.00000000	0.00000000
C	1.41534894	0.00000000	0.00000000
C	2.12116975	1.22677289	0.00000000
C	1.41540617	2.44730804	-0.12378789
C	0.00005625	2.44730824	-0.12378792
C	-0.70576358	1.22053515	-0.12378789
S	-0.88295697	-1.56028298	0.14593914
S	2.33354367	-1.54659491	0.01245286
S	3.91382166	1.25415947	0.14428597
S	2.29836315	4.00759101	-0.26972702
S	-0.91813750	3.99390295	-0.13624074
S	-2.49841547	1.19314851	-0.26807485
C	-1.78536028	-1.33719251	1.68301854
C	-1.16418238	-0.84978551	2.84121778
C	-3.11758748	-1.76517154	1.73548920
C	-1.88230371	-0.77510007	4.03441658
H	-0.12403948	-0.53958261	2.80892821
C	-3.82036285	-1.71063422	2.94011054
H	-3.60152781	-2.12622966	0.83297449
C	-3.20888448	-1.20963219	4.09002349
H	-1.39696287	-0.39158862	4.92823325
H	-4.85377412	-2.04539462	2.97289849
H	-3.76146639	-1.15746344	5.02404039
C	1.82389675	-2.29723580	-1.53781338
C	1.53865495	-3.66814176	-1.54568257
C	1.80788801	-1.57558170	-2.73939751
C	1.24515107	-4.31222715	-2.74856031
H	1.53507519	-4.22131616	-0.61128706
C	1.48847664	-2.22255828	-3.93289116
H	2.05181107	-0.51744615	-2.73961405
C	1.21188709	-3.59189527	-3.94322630
H	1.02557116	-5.37658742	-2.74644387
H	1.47270761	-1.65678611	-4.86089822
H	0.97196103	-4.09311584	-4.87685502
C	4.16988667	0.52172223	1.76430883
C	3.43356581	0.92920950	2.88531381
C	5.20888175	-0.40510005	1.91361429
C	3.72664607	0.39445095	4.13955764

H	2.64308447	1.66568623	2.77624402
C	5.51160122	-0.91543829	3.17689269
H	5.76656593	-0.73190429	1.04108736
C	4.76843371	-0.52393239	4.29117418
H	3.14907275	0.71044810	5.00448650
H	6.31996005	-1.63378897	3.28464964
H	4.99847303	-0.93119174	5.27182133
C	3.20076743	3.78450034	-1.80680639
C	4.53299365	4.21247957	-1.85927709
C	2.57958856	3.29709355	-2.96500567
C	5.23576882	4.15794127	-3.06389839
H	5.01693476	4.57353651	-0.95676230
C	3.29770989	3.22240811	-4.15820447
H	1.53944586	2.98689163	-2.93271614
C	4.62429163	3.65694002	-4.21381134
H	6.26918108	4.49270147	-3.09668630
H	2.81237003	2.83889646	-5.05202109
H	5.17687256	3.60477147	-5.14782829
C	-0.40849058	4.74454384	1.41402550
C	-0.39248302	4.02288896	2.61560963
C	-0.12324881	6.11544985	1.42189568
C	-0.07307067	4.66986534	3.80910331
H	-0.63640510	2.96475320	2.61582620
C	0.17025608	6.75953499	2.62477246
H	-0.11966905	6.66862425	0.48750017
C	0.20351885	6.03920238	3.81943946
H	-0.05730164	4.10409317	4.73711037
H	0.38983498	7.82389551	2.62265698
H	0.44344494	6.54042289	4.75306718
C	-2.75448048	1.92558575	-1.88809771
C	-2.01815945	1.51809951	-3.00910174
C	-3.79347539	2.85240907	-2.03740222
C	-2.31123971	2.05285806	-4.26334557
H	-1.22767810	0.78162278	-2.90003195
C	-4.09619584	3.36274751	-3.30068066
H	-4.35115977	3.17921232	-1.16487525
C	-3.35302735	2.97124141	-4.41496211
H	-1.73366638	1.73686091	-5.12827443
H	-4.90455487	4.08109721	-3.40843757
H	-3.58306667	3.37850076	-5.39560925

HPTB·Pb$(ClO_4)^+$: G_{MeCN} = -4772.264337 au

Pb	0.00000000	0.00000000	0.00000000
C	4.46213390	0.00000000	0.00000000
C	5.50645840	0.95581119	0.00000000
C	5.50002232	1.99677796	-0.96331516
C	4.57583001	1.95901696	-2.04079097
C	3.58209135	0.95180636	-2.08175248
C	3.55926789	-0.05465714	-1.08745183
S	4.26726697	-1.12585079	1.39340694
S	6.82674370	0.88889497	1.20875245
S	6.63281511	3.37551352	-0.83657572
S	4.58218784	3.20288964	-3.33417315
S	2.34739043	0.96597270	-3.39541264
S	2.39964285	-1.44113665	-1.10053169
C	2.70382437	-0.54875649	2.06865039
C	2.51266859	0.79150631	2.45033555
C	1.69215509	-1.49125247	2.33607436
C	1.33278757	1.17790601	3.09404041
H	3.29769872	1.52041835	2.27165086
C	0.51563288	-1.09924611	2.99750262
H	1.83730008	-2.52942106	2.05186961
C	0.33407956	0.23703094	3.37787446
H	1.20656481	2.21167151	3.40308208
H	-0.24453978	-1.84150135	3.22481068
H	-0.56889762	0.53597812	3.90145943
C	7.40447407	-0.80816031	1.05679883
C	7.62941021	-1.53757923	2.23110383
C	7.75682859	-1.35115730	-0.18685857
C	8.20331023	-2.80815801	2.15839118
H	7.35234322	-1.11419785	3.19175650
C	8.30558937	-2.63184746	-0.25067935
H	7.61596610	-0.77009739	-1.09342179
C	8.53427237	-3.36038043	0.91984342
H	8.38138235	-3.36898234	3.07139394
H	8.57564438	-3.05286339	-1.21518285
H	8.97415024	-4.35184866	0.86595929
C	6.33745613	3.98014028	0.83177530
C	5.04543870	4.28626537	1.28232750
C	7.44545658	4.27117551	1.63642748
C	4.86723999	4.85520180	2.54350956
H	4.18962558	4.09640627	0.64071050
C	7.25919681	4.86330196	2.88723990
H	8.44415081	4.02686347	1.28792716
C	5.97279496	5.14874795	3.34685028
H	3.86535732	5.09562579	2.88979888
H	8.12252062	5.09047634	3.50587608
H	5.83129454	5.60395615	4.32264012
C	6.26007947	3.15259251	-3.97773225
C	6.90994383	4.37040760	-4.21138491
C	6.86380211	1.94626510	-4.35526702
C	8.16334409	4.37709478	-4.82520301
H	6.44238591	5.30152159	-3.90652229
C	8.12921159	1.96286118	-4.94199815
H	6.34695927	1.00418388	-4.19793630
C	8.77828047	3.17616850	-5.18375666
H	8.66398464	5.32319257	-5.00942681
H	8.60069342	1.02659203	-5.22734925
H	9.75816817	3.18478691	-5.65174729
C	0.93643831	1.66865152	-2.55609967
C	-0.32506559	1.07122333	-2.78194064
C	1.00902039	2.81949209	-1.74912340
C	-1.48996110	1.63771058	-2.23244173
H	-0.39583865	0.18882926	-3.41182392
C	-0.15146744	3.36480206	-1.19245047
H	1.96675274	3.30087700	-1.58002200
C	-1.40366621	2.78260566	-1.43086807
H	-2.45152035	1.17148124	-2.42691050
H	-0.07919960	4.26352393	-0.58664195
H	-2.30243473	3.22024039	-1.00809663
C	2.47252584	-2.17491089	-2.74523755
C	3.70874098	-2.36727736	-3.37036913
C	1.29294875	-2.67636050	-3.30251522
C	3.75108874	-3.03594958	-4.59379877
H	4.62290680	-2.00331134	-2.91227039
C	1.35687337	-3.36092098	-4.51839390
H	0.34085698	-2.55162542	-2.79583956
C	2.57895035	-3.53211662	-5.17010241
H	4.70645641	-3.18116743	-5.08957110
H	0.44414433	-3.75452509	-4.95584279
H	2.62063634	-4.05810371	-6.11893973
O	-2.52483725	-0.57987749	0.43674213
Cl	-2.53286728	-1.83506147	-0.43286281
O	-1.00157289	-1.95455623	-0.84347082

O	-3.31680693	-1.62474188	-1.65260940
O	-2.90497206	-3.01978354	0.33354555

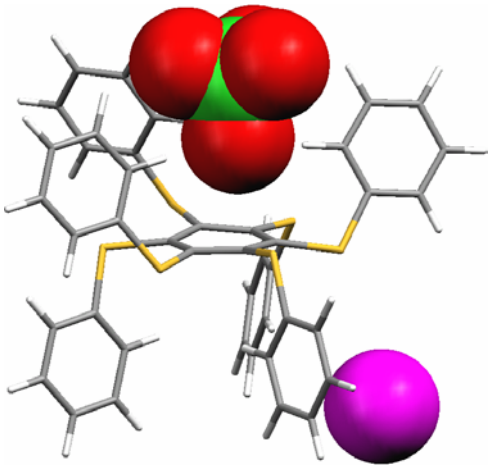
HPTB·Hg$(ClO_4)^+$: G_{MeCN} = -4922.266626 au

Hg	0.00000000	0.00000000	0.00000000
C	3.49168101	0.00000000	0.00000000
C	3.89004025	1.35254774	0.00000000
C	3.51960237	2.18570146	-1.09126523
C	2.85721906	1.62092245	-2.21639816
C	2.50577022	0.24785971	-2.21383830
C	2.91005885	-0.59070984	-1.14644969
S	3.62730801	-1.01957374	1.47743992
S	4.86200466	2.03222959	1.34705505
S	3.87531940	3.93524345	-1.09562687
S	2.41664657	2.62649155	-3.63466686
S	1.58386840	-0.40936532	-3.62084120
S	2.84634658	-2.39277177	-1.27031463
C	2.05649266	-0.74889214	2.22920733
C	1.24484333	0.42257387	2.02984602
C	1.63963674	-1.70634214	3.17063230
C	0.09272928	0.62458629	2.86166586
H	1.70168872	1.30089669	1.57560070
C	0.49135963	-1.49649731	3.92919373
H	2.22871846	-2.60692155	3.31672601
C	-0.28760737	-0.33369154	3.78275106
H	-0.47088603	1.54647366	2.75140774
H	0.19667000	-2.25029308	4.65405767
H	-1.16775359	-0.18229028	4.39841686
C	6.25083766	0.88874602	1.41942636
C	6.64083117	0.39342399	2.66930650
C	7.01589466	0.60497452	0.27903447
C	7.79151114	-0.39098295	2.77551902
H	6.04768972	0.61899688	3.55036426
C	8.14941307	-0.20070869	0.39219676
H	6.73780712	1.02644001	-0.68247550
C	8.54116112	-0.69715880	1.63894989
H	8.09450657	-0.76918633	3.74757044
H	8.74318964	-0.41899745	-0.49112905
H	9.43204518	-1.31227659	1.72372792
C	3.11775410	4.52700920	0.42684016
C	1.74396686	4.35986363	0.65377016
C	3.89195186	5.29495088	1.30543889
C	1.15746967	4.93537895	1.78301231
H	1.12779815	3.81645464	-0.05587447
C	3.29044713	5.88530011	2.41844342
H	4.95430764	5.42174028	1.12206636
C	1.92819904	5.69982734	2.66348355
H	0.09190524	4.80659526	1.94901954
H	3.89085752	6.48510464	3.09641416
H	1.46513862	6.16051391	3.53136249
C	4.01273445	3.21348462	-4.22279270
C	4.12109509	4.56365964	-4.57713405
C	5.08501124	2.33767369	-4.43784304
C	5.30338346	5.03347565	-5.15114639
H	3.29132810	5.23988509	-4.39627113
C	6.27153683	2.82472944	-4.98671778
H	4.99391185	1.28484165	-4.18636705
C	6.38157158	4.16927128	-5.34994436
H	5.38373683	6.08020752	-5.42957037
H	7.10521866	2.14700693	-5.14823390
H	7.30322744	4.54062065	-5.78807394
C	-0.07813787	-0.63331115	-3.00479924
C	-0.41758006	-1.45738059	-1.88123295
C	-1.10643635	-0.07056779	-3.76590864
C	-1.79319839	-1.69832770	-1.58195503
H	0.33431727	-2.16338458	-1.52709503
C	-2.44490669	-0.29800924	-3.42653059
H	-0.86190426	0.56493732	-4.61063706
C	-2.79469340	-1.10393943	-2.33487841
H	-2.04323916	-2.36869402	-0.76435694
H	-3.22487716	0.17475024	-4.01608794
H	-3.83781309	-1.26862106	-2.08790310
C	4.01491442	-2.70241297	-2.60612271
C	5.33483704	-2.23924398	-2.52884957
C	3.60496393	-3.50493961	-3.67664113
C	6.23489873	-2.56399678	-3.54425706
H	5.66045763	-1.64274151	-1.68175202
C	4.52168682	-3.84370623	-4.67392799
H	2.57999365	-3.85758352	-3.73165471
C	5.83256800	-3.36826672	-4.61406444
H	7.25836649	-2.20410921	-3.48867252
H	4.20467035	-4.46956080	-5.50292353
H	6.54082000	-3.62725385	-5.39541255
O	-0.68186074	2.22928002	-0.62223962
Cl	-2.05695064	2.31679717	0.10610549
O	-2.34418454	0.87564533	0.52953790
O	-3.07470935	2.80402728	-0.82898820
O	-1.90262712	3.16743249	1.30464872

Hg·HPTB·$(ClO_4)^+$ (C_3): G_{MeCN} = -4922.326257 au

Hg	0.00000000	0.00000000	0.00000000
Cl	10.99418600	0.00000000	0.00000000
O	10.46322802	1.41042289	0.00000000
O	10.46322802	-0.70521145	1.22146206
O	10.46322802	-0.70521145	-1.22146206
O	12.47014800	-0.00000000	0.00000000
C	7.26791004	-0.53777320	-1.29471192
C	7.28333899	-1.39350409	-0.18160684
C	7.26791004	-0.85236681	1.11308121
C	7.28333899	0.53947591	1.29761335
C	7.26791004	1.39014001	0.18163070
C	7.28333899	0.85402817	-1.11600653
S	7.26108910	-1.22463337	-2.94165085
S	7.01005498	-3.14837811	-0.41630367
S	7.26108909	-1.93522768	2.53138903
S	7.01005498	1.21365950	2.93472724
S	7.26108910	3.15986104	0.41026181
S	7.01005498	1.93471859	-2.51842359
C	5.53169611	-1.35422640	-3.38196590
C	4.46851908	-1.24117729	-2.47869296

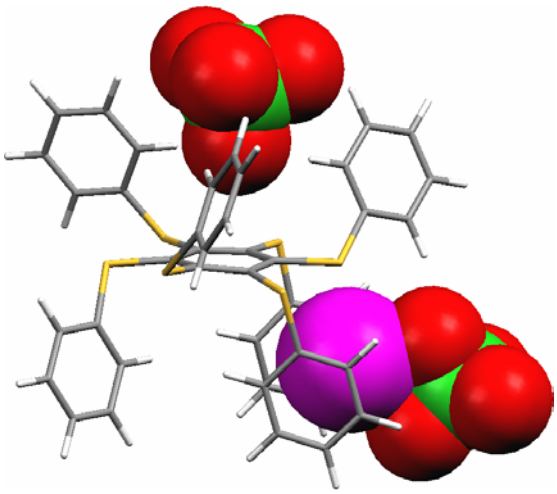
C	5.28597616	-1.62606854	-4.73721889
C	3.16060610	-1.39613332	-2.93807299
H	4.65084205	-1.04569818	-1.42709697
C	3.97447617	-1.78124056	-5.18133592
H	6.11197818	-1.71052562	-5.43795485
C	2.90834914	-1.66543046	-4.28596697
H	2.33558807	-1.31440524	-2.23547803
H	3.78770721	-1.98990967	-6.23037591
H	1.88763915	-1.78711848	-4.63513800
C	8.55548797	-4.01564914	-0.54712552
C	8.43870297	-5.29343720	-1.13129439
C	9.78345095	-3.54344010	-0.06740352
C	9.56985496	-6.09318622	-1.23995027
H	7.48019798	-5.64595422	-1.50181439
C	10.90592594	-4.35861813	-0.19416339
H	9.87593494	-2.56747206	0.39164338
C	10.80659595	-5.62679319	-0.77554127
H	9.49031997	-7.07636026	-1.69358317
H	11.86213594	-3.99290110	0.16685861
H	11.68929295	-6.25250421	-0.86716417
C	5.53169611	-2.25175519	2.86377740
C	4.46851908	-1.52602242	2.31423753
C	5.28597616	-3.28951763	3.77682609
C	3.16060609	-1.84637919	2.67812341
H	4.65084205	-0.71305313	1.61914967
C	3.97447617	-3.59654825	4.13326753
H	6.11197818	-3.85414423	4.20033605
C	2.90834914	-2.87904105	3.58528856
H	2.33558807	-1.27877815	2.25604734
H	3.78770721	-4.40070898	4.83850027
H	1.88763915	-3.12058802	3.86525899
C	8.55548797	1.53399997	3.75121691
C	8.43870297	1.66698891	5.14989827
C	9.78345095	1.71334689	3.10241090
C	9.56985496	1.97276468	5.89682918
H	7.48019798	1.52236769	5.64044697
C	10.90592594	2.01115863	3.87175571
H	9.87593494	1.62290915	2.02767433
C	10.80659595	2.14175815	5.26071647
H	9.49031997	2.07149408	6.97509933
H	11.86213594	2.14095434	3.37452448
H	11.68929295	2.37526590	5.84840956
C	5.53169611	3.60598158	0.51818848
C	4.46851908	2.76719971	0.16445541
C	5.28597616	4.91558616	0.96039278
C	3.16060610	3.24251250	0.25994957
H	4.65084205	1.75875131	-0.19205271
C	3.97447617	5.37778881	1.04806838
H	6.11197818	5.56466984	1.23761878
C	2.90834914	4.54447150	0.70067840
H	2.33558807	2.59318338	-0.02056932
H	3.78770721	6.39061864	1.39187562
H	1.88763915	4.90770649	0.76987899
C	8.55548797	2.48164916	-3.20409141
C	9.78345095	1.83009320	-3.03500739
C	8.43870297	3.62644827	-4.01860389
C	10.90592594	2.34745949	-3.67759233
H	9.87593494	0.94456291	-2.41931772
C	9.56985496	4.12042153	-4.65687893
H	7.48019798	4.12358652	-4.13863259
C	10.80659595	3.48503502	-4.48517521
H	11.86213594	1.85194675	-3.54138310
H	9.49031997	5.00486617	-5.28151617
H	11.68929295	3.87723830	-4.98124540



Hg·HPTB·(ClO_4): G_{MeCN} = -4922.533753 au

Hg	0.00000000	0.00000000	0.00000000
Cl	9.93936965	0.00000000	0.00000000
O	9.85980224	1.49706512	0.00000000
O	10.96424887	-0.44380684	0.99582696
O	8.58142598	-0.53427673	0.43191515
O	10.26276964	-0.50902529	-1.35483209
C	5.72024827	-1.25152004	1.26260291
C	6.21756492	-1.54473606	2.54064611
C	6.32872371	-0.51500738	3.49948040
C	6.06056173	0.82352947	3.10828854
C	5.43400113	1.08689834	1.86208126
C	5.28491685	0.03913767	0.93207590
S	5.78256205	-2.50496575	-0.00837140
S	6.52489100	-3.27566334	2.85197097
S	6.80600950	-0.87285467	5.19075301
S	6.44029909	2.19577915	4.18816195
S	4.84985910	2.72455634	1.42844967
S	4.48462260	0.20963424	-0.65367774
C	4.18804495	-3.29953148	0.03329625
C	3.24388171	-3.11953634	1.05359266
C	3.91637586	-4.17390881	-1.03244571
C	2.03304325	-3.81050583	0.99949624
H	3.45155952	-2.45499604	1.88572479
C	2.70389733	-4.85743704	-1.07417119

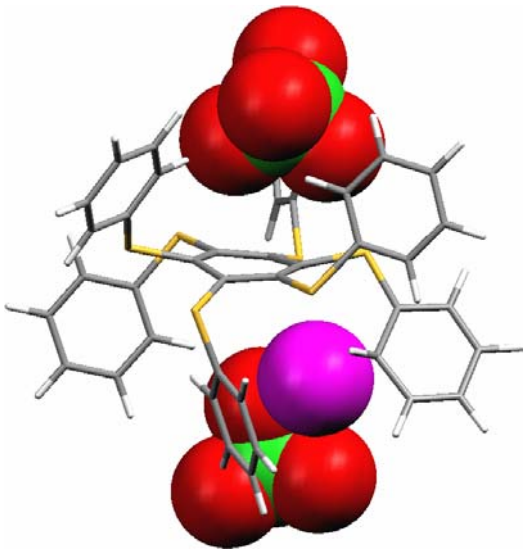
H	4.64826731	-4.31111199	-1.82377160
C	1.75752293	-4.67781759	-0.06092309
H	1.30664141	-3.67492090	1.79584750
H	2.49744880	-5.53006922	-1.90158391
H	0.81347532	-5.21345022	-0.09531323
C	8.23528355	-3.43518078	3.32049002
C	8.53588606	-4.50573107	4.18015609
C	9.24646972	-2.62036245	2.79648497
C	9.86334998	-4.74830154	4.52390952
H	7.74038501	-5.13031941	4.57718278
C	10.56890784	-2.87420439	3.15709421
H	9.02175502	-1.81632563	2.10289869
C	10.88006982	-3.93140859	4.01687951
H	10.10337224	-5.57141050	5.19134505
H	11.34370750	-2.24276662	2.73506849
H	11.91440011	-4.12566700	4.28693030
C	5.42897565	-1.88901222	5.74098795
C	4.09612534	-1.51773048	5.51655153
C	5.71792988	-3.02039047	6.51428399
C	3.06331183	-2.29560663	6.04050526
H	3.86962734	-0.62057562	4.94808930
C	4.67749538	-3.77826074	7.05505856
H	6.75187858	-3.30757379	6.68178030
C	3.34909957	-3.42464836	6.81287271
H	2.03101304	-2.00550895	5.86218455
H	4.90828172	-4.65383739	7.65589819
H	2.54110254	-4.02067508	7.22768788
C	8.20079944	1.96853965	4.48503221
C	8.67353661	2.15799287	5.79009741
C	9.09229527	1.71969674	3.43390081
C	10.04559140	2.10134476	6.03799231
H	7.97348195	2.33721994	6.60089631
C	10.45996009	1.63286618	3.69962696
H	8.74154392	1.59266635	2.41535621
C	10.93765333	1.83117362	4.99722320
H	10.41357596	2.25179572	7.04958841
H	11.13394040	1.40999154	2.87871536
H	12.00412377	1.77407443	5.19797482
C	3.62027814	3.03835748	2.70255572
C	2.62753879	2.10171368	3.02284844
C	3.61076872	4.30021284	3.30854489
C	1.64420906	2.42501235	3.95845773
H	2.62184053	1.12895000	2.53983232
C	2.60762096	4.62409065	4.22446867
H	4.39095871	5.01698046	3.07136234
C	1.62733224	3.68808444	4.55652560
H	0.88159638	1.69241533	4.20988191
H	2.60506558	5.60582594	4.68992551
H	0.85485901	3.93910722	5.27781461
C	5.44367813	1.39874943	-1.56701917
C	6.81252771	1.59554131	-1.34179206
C	4.76972740	2.09198164	-2.58724984
C	7.50484589	2.50969427	-2.13517728
H	7.34436767	1.03254728	-0.58253237
C	5.47846513	2.99265639	-3.37659540
H	3.70635095	1.93670614	-2.74793012
C	6.84380662	3.20597818	-3.15028015
H	8.56537624	2.64667291	-1.95017150
H	4.96298074	3.53632924	-4.16340948
H	7.39020552	3.91172611	-3.76963129



$(ClO_4)\cdot HPTB\cdot Pb(ClO_4)$: G_{MeCN} = -5533.265724 au

Pb	0.00000000	0.00000000	0.00000000
Cl	8.30193086	0.00000000	0.00000000
O	6.90987958	0.61317678	0.00000000
O	8.97620175	0.33751223	1.28700165
O	8.16730758	-1.48220665	-0.13690380
O	9.07181560	0.55517021	-1.15020781
C	3.67356209	1.69278008	1.38778010
C	4.31102131	2.94939919	1.25985688
C	4.50957705	3.49569348	-0.03300498
C	4.25675385	2.71179005	-1.18598346
C	3.69278400	1.42064855	-1.04783322
C	3.43994970	0.89997621	0.24126670
S	3.10321593	1.12404791	3.00092468
S	4.81780576	3.90242338	2.68486442
S	5.05909803	5.18989605	-0.22461997
S	4.54639370	3.33129663	-2.84269618
S	3.29104020	0.45871794	-2.51642892
S	2.75176578	-0.74878655	0.56015128
C	1.33137292	1.31412028	2.78671923
C	0.75644161	2.53227232	2.37820536
C	0.48473406	0.24238585	3.13706398
C	-0.63333689	2.67457603	2.33269256
H	1.39698326	3.37190088	2.12522721
C	-0.91176634	0.39878538	3.10328198
H	0.92031176	-0.69944247	3.45870189
C	-1.47353402	1.61548758	2.69988919

H	-1.06101913	3.62698544	2.03181290
H	-1.55069833	-0.43092145	3.39257470
H	-2.55223150	1.73608344	2.67671101
C	5.69504465	2.71081255	3.70757748
C	5.48758759	2.77999544	5.09230891
C	6.64631872	1.83498108	3.17050884
C	6.23913869	1.96724989	5.94083867
H	4.74106274	3.45743348	5.49741786
C	7.37335738	1.00806182	4.03020018
H	6.83058181	1.77939715	2.10225612
C	7.17648000	1.07617238	5.41105891
H	6.08186687	2.02306912	7.01495144
H	8.10328750	0.33404181	3.59341863
H	7.75495361	0.43913325	6.07476165
C	3.77135140	6.10418970	0.63270660
C	2.40930899	5.87537454	0.38848745
C	4.15627393	7.15520807	1.47444462
C	1.44605063	6.67765296	1.00075293
H	2.11030319	5.08123211	-0.28964453
C	3.18702325	7.96870601	2.06466297
H	5.21016084	7.32392649	1.67368627
C	1.83111027	7.72924374	1.83713173
H	0.39162654	6.49790864	0.80431742
H	3.49546637	8.78223178	2.71544477
H	1.07908044	8.35902955	2.30396995
C	6.25434809	3.89527244	-2.82974225
C	6.54287074	5.09670072	-3.49010860
C	7.27762486	3.10855089	-2.28986710
C	7.87022610	5.50754466	-3.61255162
H	5.73806677	5.70527199	-3.89228651
C	8.59947164	3.54669151	-2.39610722
H	7.06851498	2.17098886	-1.78475520
C	8.89799199	4.73794130	-3.06060659
H	8.09765663	6.43749796	-4.12725065
H	9.37917331	2.92696516	-1.96493999
H	9.92982748	5.06690062	-3.15018300
C	1.53761665	0.75927181	-2.66211055
C	0.69581419	-0.35188970	-2.90296697
C	0.96332688	2.04469247	-2.61155428
C	-0.68290699	-0.17085640	-3.11533166
H	1.12959638	-1.34711633	-2.95057624
C	-0.40963947	2.21269201	-2.80911845
H	1.59629808	2.91023005	-2.44468047
C	-1.23852539	1.11198363	-3.06356911
H	-1.31198440	-1.03714343	-3.29865199
H	-0.83178859	3.21341339	-2.78183920
H	-2.30323800	1.25101685	-3.22220252
C	3.58440127	-1.96579226	-0.48240790
C	4.97456143	-1.93196299	-0.60380351
C	2.81683706	-3.01029675	-1.00906814
C	5.60327862	-2.95899001	-1.31140750
H	5.57415718	-1.12984948	-0.18166867
C	3.46895062	-4.03465210	-1.69870104
H	1.74006819	-3.04432680	-0.87182593
C	4.85629289	-4.00432180	-1.85909062
H	6.68352781	-2.91826243	-1.40556581
H	2.88549749	-4.85350265	-2.11068316
H	5.35578158	-4.80159939	-2.40229356
O	-2.51923185	-1.16036792	-0.09943256
Cl	-1.94794073	-2.56043411	-0.12638606
O	-0.38949282	-2.31821444	0.06189907
O	-2.14763782	-3.19384008	-1.43626983
O	-2.42141824	-3.36432864	1.00118035



$(ClO_4)\cdot HPTB\cdot Hg(ClO_4)$: G_{MeCN} = -5683.264822 au

Hg	0.00000000	0.00000000	0.00000000
Cl	7.25256932	0.00000000	0.00000000
O	7.76335401	1.40976009	0.00000000
O	6.20613914	-0.13965568	1.08514381
O	6.60461310	-0.29466022	-1.32077169
O	8.35763747	-0.95726512	0.25991401
C	3.57566175	-0.48101318	-2.26453851
C	3.27087621	-0.72605460	-0.91150058
C	3.16212504	0.36169169	0.00407471
C	3.19980775	1.70081950	-0.46078238
C	3.30552837	1.91543442	-1.85428717
C	3.69284407	0.85787067	-2.71465510
S	3.84548004	-1.86779298	-3.35565706
S	2.77276240	-2.34345379	-0.30683963
S	3.25113770	-0.08565669	1.73734557
S	2.98191214	3.16032970	0.57355548
S	2.87080565	3.52070117	-2.53705771
S	4.27136414	1.17458819	-4.36805151

C	2.62965249	-1.61027773	-4.65789527
C	1.26554846	-1.47784116	-4.36537676
C	3.05800669	-1.65804263	-5.99016408
C	0.34052781	-1.35892708	-5.40303325
H	0.92112791	-1.49053544	-3.33682108
C	2.12263622	-1.56546522	-7.02299763
H	4.11643708	-1.75320496	-6.21239535
C	0.76625586	-1.40629140	-6.73328857
H	-0.71441586	-1.25018246	-5.16529076
H	2.45962229	-1.60375051	-8.05535069
H	0.04287693	-1.32487068	-7.53987603
C	4.16446915	-3.47370667	-0.42568088
C	3.90821297	-4.73628561	-0.97741500
C	5.42625133	-3.14981698	0.07946080
C	4.93394989	-5.67972735	-1.02193816
H	2.92710965	-4.96758852	-1.38117239
C	6.45309092	-4.09164305	-0.00694760
H	5.61668617	-2.18038313	0.52464168
C	6.20840531	-5.35554185	-0.54716798
H	4.74136531	-6.66041572	-1.44853774
H	7.44091021	-3.81655560	0.34981607
H	7.00972353	-6.08729232	-0.60368422
C	1.72361932	0.27018084	2.44172546
C	0.65542428	1.05602526	1.81973489
C	1.51761222	-0.25055841	3.74342831
C	-0.55575116	1.29199819	2.60224328
H	1.03496248	1.94675291	1.29275476
C	0.32679986	-0.04077251	4.40654867
H	2.30271628	-0.84062902	4.20719801
C	-0.72187488	0.73952422	3.83946997
H	-1.31623901	1.93822144	2.17303437
H	0.18787332	-0.47925559	5.39068429
H	-1.63180242	0.91131468	4.40509861
C	4.11963146	3.02230097	1.96011567
C	3.61352755	3.30202153	3.23756869
C	5.48370993	2.79177872	1.76590871
C	4.48483739	3.34192213	4.32667237
H	2.55289706	3.49468161	3.37738311
C	6.33796219	2.79846567	2.86899529
H	5.89168212	2.58395093	0.78432928
C	5.84555244	3.07948567	4.14475448
H	4.09758130	3.56744823	5.31687650
H	7.38857005	2.57908678	2.70876168
H	6.51939005	3.09510022	4.99696091
C	1.12011001	3.52339972	-2.11453186
C	0.27867396	2.45790779	-2.48194506
C	0.57474123	4.65022980	-1.48739949
C	-1.09086883	2.51811160	-2.19968719
H	0.68250190	1.61035333	-3.02860616
C	-0.79688643	4.70972059	-1.22071468
H	1.22464843	5.47218560	-1.20296870
C	-1.63019749	3.64449804	-1.56553462
H	-1.74125847	1.70913564	-2.52104516
H	-1.20983938	5.59195911	-0.73889215
H	-2.69687075	3.69551385	-1.36597201
C	5.42502007	2.53469556	-4.12081108
C	6.45134121	2.43796993	-3.17122725
C	5.35027451	3.63619418	-4.98300969
C	7.38467892	3.47036697	-3.07033901
H	6.53248157	1.56898246	-2.52507336
C	6.30868248	4.64691972	-4.89065483
H	4.54618552	3.70343878	-5.70992388
C	7.32016050	4.56997942	-3.93013021
H	8.16733960	3.39210395	-2.32136057
H	6.25438017	5.50044309	-5.56126877
H	8.05784988	5.36447316	-3.85466579
O	-0.76459868	-1.13231169	-1.65710269
Cl	-2.37565715	-1.29887295	-1.56117387
O	-2.75695738	-0.59101710	-0.30162709
O	-2.64547618	-2.73731398	-1.50690214
O	-2.91862618	-0.63988085	-2.75934922

Calculated structures: cartesian coordinates (in Å) and energies computed for compounds **5**, **7** and their complexes with $M(ClO_4)_2$ (M: Pb, Hg)**.-**

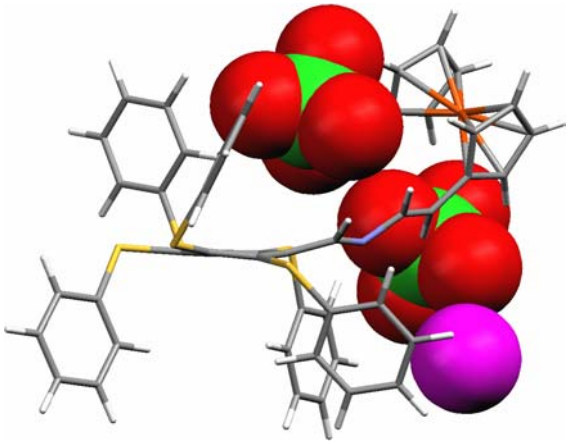
Compound **5**: G_{MeCN} = -5199.395957 au

C	0.00000000	0.00000000	0.00000000
N	1.28159655	0.00000000	0.00000000
C	1.93517882	1.22523666	0.00000000
C	3.28394924	1.28074797	-0.01053150
H	-0.58669188	0.92805388	0.00236874
H	1.33134742	2.13926081	0.02620534
H	3.81818688	0.33266516	-0.01448828
C	4.09212596	2.49026835	0.01576736
C	5.52074673	2.51605663	0.17942126
C	5.95595954	3.87191119	0.18939153
C	4.80728415	4.70186533	0.01784881
C	3.66502141	3.85849798	-0.10176539
H	6.15020567	1.64152208	0.28635166
H	6.97812942	4.21201920	0.29242955
H	4.80488759	5.78300137	-0.03388568
H	2.64769422	4.19353640	-0.25530583
Fe	5.01505032	3.43159400	-1.58052558
C	4.79756545	2.24553409	-3.24271793
C	4.01564722	3.43309190	-3.37098875
C	4.89894025	4.55271732	-3.29595820
C	6.22563165	4.05652958	-3.11900478
C	6.16289747	2.63061141	-3.08566193
H	4.41769180	1.23204702	-3.23411851
H	2.94024009	3.47776221	-3.48491978
H	4.61170605	5.59494900	-3.34844367
H	7.12045295	4.65638191	-3.01418130
H	7.00149818	1.95967718	-2.95177935
C	-0.76916015	-1.27571571	0.04717659
C	-1.64000649	-1.48302648	1.13405408
C	-2.37456989	-2.68468967	1.26097884
C	-2.21524611	-3.69667638	0.28622391
C	-1.29633495	-3.51639568	-0.77979668
C	-0.64278426	-2.27329590	-0.94606705
S	-1.66386026	-0.21232567	2.40924982
C	-3.30898705	0.49274329	2.27623626
C	-3.91280026	0.95328231	3.45334325
C	-5.15265676	1.58962192	3.39717032
C	-5.80757982	1.75319622	2.17519146
C	-5.20832023	1.28520754	1.00433956
C	-3.95825604	0.66713560	1.04750050
H	-3.41764752	0.80218169	4.40817485
H	-5.61405853	1.94350593	4.31528617
H	-6.77847845	2.23901136	2.13580929
H	-5.70956377	1.41049775	0.04800547
H	-3.48995183	0.32232372	0.13036553
S	-3.51471530	-2.86510158	2.63451438
C	-2.82731664	-4.23507552	3.56827340
C	-3.72457382	-5.12224533	4.17619668
C	-3.24546557	-6.14498027	4.99507324
C	-1.87314420	-6.30407426	5.19477091
C	-0.97990568	-5.42433528	4.57985643
C	-1.45060287	-4.38332003	3.77942802
H	-4.79064263	-5.01711945	3.99712834
H	-3.94830438	-6.82892563	5.46350411
H	-1.50188264	-7.10859467	5.82347259
H	0.09008561	-5.53780327	4.73355723
H	-0.75284456	-3.68753196	3.32377029
S	-3.15556652	-5.21963274	0.44415734
C	-4.14632790	-5.23227660	-1.05369729
C	-4.82803382	-4.09421728	-1.50478222
C	-5.65430102	-4.17809346	-2.62514180
C	-5.82981820	-5.39665233	-3.28478155
C	-5.16311639	-6.53299890	-2.82440821
C	-4.31423608	-6.45274090	-1.71979812
H	-4.71644916	-3.15157724	-0.97770247
H	-6.17498756	-3.28994317	-2.97387275
H	-6.48121263	-5.45907093	-4.15207523
H	-5.28863668	-7.48409362	-3.33506953
H	-3.77205068	-7.32989656	-1.37925543
S	-1.03305047	-4.85541495	-1.94500929
C	0.74155263	-5.11896478	-1.85489179
C	1.42713994	-5.37512821	-3.04897650
C	2.78400612	-5.69923805	-3.01703637
C	3.46787712	-5.74700997	-1.80141524
C	2.78456041	-5.48200074	-0.61242383
C	1.42271953	-5.18336836	-0.63233323
H	0.90062531	-5.30848683	-3.99648555
H	3.30921995	-5.89794956	-3.94752165
H	4.52714685	-5.98781306	-1.77977942
H	3.30954854	-5.52013794	0.33840303
H	0.88956369	-5.00103581	0.29550329
S	0.31562510	-1.97509483	-2.43898254
C	-0.38521876	-0.43127851	-3.02437592
C	0.48878167	0.54059239	-3.52786237
C	-0.01867708	1.70872143	-4.10022305
C	-1.39566228	1.92774945	-4.15171217
C	-2.26767115	0.96101629	-3.64360739
C	-1.77008815	-0.22128814	-3.09709063
H	1.56106882	0.38286242	-3.46267428
H	0.66762342	2.45253832	-4.49700116
H	-1.78842223	2.84187253	-4.58817537
H	-3.34217020	1.11825585	-3.69188369
H	-2.45175803	-0.98519717	-2.73542652

Complex **5**·$Pb(ClO_4)_2$: G_{MeCN} = -6724.542805 au

C	0.00000000	0.00000000	0.00000000
N	1.29719938	0.00000000	0.00000000
C	1.92182336	1.26732907	0.00000000
C	3.25548646	1.45092333	-0.04053268
H	-0.53626300	0.95793643	-0.01121565
H	1.22927476	2.10634695	0.03008745
H	3.92384453	0.59377196	-0.06218232
C	-0.90510897	-1.18636426	-0.00275305

C	-1.53197922	-1.53469620	1.20982195
C	-2.64053873	-2.40107611	1.21360976
C	-3.06814142	-2.97797475	-0.01047244
C	-2.47646503	-2.58794591	-1.23881974
C	-1.34034066	-1.74620373	-1.21637142
S	-0.86900646	-0.78001897	2.71046393
C	0.56585389	-1.82660922	2.97690229
C	0.44491682	-3.22121233	3.11606119
C	1.57181877	-4.00197110	3.38590451
C	2.83162315	-3.40916548	3.53330622
C	2.96088542	-2.02228459	3.40857058
C	1.83489668	-1.23012768	3.12316964
H	-0.53502981	-3.68122119	3.03372471
H	1.46303693	-5.07748419	3.49419855
H	3.70632863	-4.01904141	3.73437719
H	3.93543158	-1.55452718	3.51246991
H	1.93627682	-0.15272526	3.02792587
S	-3.54543448	-2.80281059	2.70724439
C	-3.95037029	-1.20262157	3.42894241
C	-4.13053306	-1.18358917	4.81774882
C	-4.52420730	-0.00062131	5.44408359
C	-4.70870648	1.16524744	4.69733403
C	-4.51641901	1.14136468	3.31454979
C	-4.15897187	-0.04555865	2.67011432
H	-3.95703458	-2.08150401	5.40479441
H	-4.66667099	0.01039739	6.52159974
H	-4.99388119	2.08963450	5.19171050
H	-4.62716595	2.04038511	2.71606240
H	-4.01964382	-0.03314085	1.59435619
S	-4.41127451	-4.16871939	0.03340258
C	-3.68678834	-5.60570391	-0.76490371
C	-4.46536784	-6.30518386	-1.69551934
C	-3.98692648	-7.49241409	-2.25288106
C	-2.72496663	-7.97672890	-1.90522979
C	-1.94515722	-7.27454155	-0.98213737
C	-2.42665455	-6.10132839	-0.40085419
H	-5.43435250	-5.91261874	-1.98817428
H	-4.59864267	-8.03014363	-2.97198919
H	-2.35201863	-8.89638690	-2.34704118
H	-0.96768579	-7.65410561	-0.69482380
H	-1.83250992	-5.57591650	0.34117182
S	-3.21336239	-3.14652431	-2.76957814
C	-3.45575456	-1.63195269	-3.71278022
C	-3.72128691	-0.39141823	-3.12194373
C	-3.94622585	0.72189721	-3.93566202
C	-3.95150084	0.59141251	-5.32587425
C	-3.71192050	-0.65570808	-5.90794150
C	-3.44839608	-1.76720037	-5.10709085
H	-3.73025025	-0.26063612	-2.04510457
H	-4.10540461	1.68502686	-3.46041995
H	-4.13548021	1.45901818	-5.95339159
H	-3.70904411	-0.76417478	-6.98949137
H	-3.22982350	-2.72974441	-5.56179392
S	-0.46055874	-1.27417950	-2.72218075
C	0.90843705	-2.43015810	-2.64964851
C	0.71075740	-3.81592042	-2.50230435
C	1.80379872	-4.68571672	-2.51344426
C	3.10553359	-4.19864839	-2.68279237
C	3.31274005	-2.82572391	-2.83942549
C	2.22174695	-1.93946555	-2.81130703
H	-0.29628457	-4.20715813	-2.39795023
H	1.63433216	-5.75282372	-2.40018840
H	3.95157683	-4.87805298	-2.68200462
H	4.31966836	-2.43620711	-2.95485083
H	2.38108046	-0.87179345	-2.93597087
C	3.89784658	2.75525062	-0.03235082
C	5.31585077	2.96625594	0.11014525
C	5.56348291	4.36774942	0.10994832
C	4.31128883	5.03742122	-0.04589922
C	3.28665555	4.05412553	-0.14503180
H	6.05690392	2.18364624	0.21281368
H	6.53233461	4.84187301	0.19523375
H	4.16547552	6.10807856	-0.10325806
H	2.23159503	4.25263556	-0.28157718
Fe	4.65777923	3.78890146	-1.64432920
C	4.52308640	2.60484315	-3.32104658
C	3.63493094	3.71821917	-3.42597199
C	4.41764220	4.91012700	-3.34964315
C	5.78591165	4.53272193	-3.19411527
C	5.85175333	3.10623364	-3.17558201
H	4.23592395	1.56134706	-3.32850745
H	2.55903117	3.66912009	-3.53105175
H	4.03722827	5.92254098	-3.38581616
H	6.62476949	5.20906217	-3.09392771
H	6.74811731	2.51103438	-3.06003375
Pb	2.26195062	-2.25463784	0.23055998
Cl	5.54695085	-2.61583138	0.39289619
O	4.72812422	-3.86629467	0.50238127
O	4.48020923	-1.45078801	0.21566199
O	6.29055576	-2.33692164	1.62860169
O	6.38957581	-2.61522962	-0.81109922
Cl	-2.70753596	2.60180833	-0.29604240
O	-1.22499856	2.86454137	-0.18913895
O	-2.91066061	1.10222530	-0.22466276
O	-3.41658639	3.25197878	0.83717464
O	-3.21297084	3.10844967	-1.59963543



Complex **5**·$Hg(ClO_4)_2$: G_{MeCN} = -6874.625049 au

C	0.00000000	0.00000000	-0.00000000
N	1.28801481	0.00000000	-0.00000000
C	1.94730253	1.21482164	-0.00000000
C	3.29186098	1.28887172	-0.10544990
H	-0.57316251	0.91227383	0.18162110
H	1.32630430	2.11053473	-0.03062184
H	3.90065998	0.39098829	-0.08432113
C	3.97282794	2.54763342	-0.35379507
C	3.39789975	3.75503324	-0.87894801
C	4.44144953	4.70931281	-1.06533884
C	5.67712610	4.08138531	-0.70359339
C	5.38808557	2.74969904	-0.28587582
H	2.35365149	3.89518467	-1.13060891
H	4.31685626	5.72207725	-1.42565863
H	6.65935004	4.53428464	-0.73541963
H	6.09657601	1.98297588	0.00806816
Fe	4.80626101	3.09806509	-2.29744372
C	4.44286909	1.54307199	-3.73344349
C	5.83907551	1.75860756	-3.57989361
C	6.10796521	3.12290207	-3.90629690
C	4.86437159	3.74514609	-4.25681729
C	3.83442144	2.75887849	-4.14725708
H	3.91672701	0.63133109	-3.48543714
H	6.55078670	1.03192424	-3.20330322
H	7.07979077	3.59904199	-3.88802105
H	4.72718957	4.77544658	-4.55885184
H	2.76966446	2.90581697	-4.30105542
C	-0.76540592	-1.14626806	-0.47698880
C	-0.15798872	-2.07302084	-1.34726917
C	-0.92231886	-2.95054312	-2.11834692
C	-2.33315083	-2.92339070	-2.04378131
C	-2.96128304	-2.00510590	-1.16601135
C	-2.17047005	-1.20419673	-0.30424763
S	1.61044485	-2.07379510	-1.63707495
C	2.26357568	-3.20569806	-0.44918000
C	1.48828828	-3.91560578	0.48349865
C	2.12014566	-4.79358237	1.35848971
C	3.51051570	-4.96132711	1.31596309
C	4.27664345	-4.24391339	0.39292950
C	3.66064145	-3.36836316	-0.49759607
H	0.41366414	-3.77809171	0.52705538
H	1.52728802	-5.34795354	2.08058807
H	3.99321077	-5.64593670	2.00754719
H	5.35692009	-4.33971326	0.36221350
H	4.26200087	-2.79400909	-1.19545237
S	-0.01483919	-4.03732089	-3.21679343
C	-0.34102828	-3.33741663	-4.83472180
C	-0.34541105	-4.22591307	-5.91983370
C	-0.53204651	-3.72934509	-7.20897297
C	-0.72596449	-2.36047656	-7.41542326
C	-0.72266162	-1.48333841	-6.32824005
C	-0.51981881	-1.96227613	-5.03423727
H	-0.21644874	-5.29172797	-5.75454686
H	-0.53800215	-4.41603580	-8.05086675
H	-0.87853684	-1.97987970	-8.42141557
H	-0.86740622	-0.41644876	-6.46845592
H	-0.49566031	-1.25650858	-4.21188667
S	-3.25845214	-4.00314851	-3.12850704
C	-4.24151614	-4.98703173	-1.99097110
C	-5.58093916	-5.22525091	-2.32297027
C	-6.35281565	-6.07322831	-1.52727870
C	-5.80218680	-6.66683132	-0.39013656
C	-4.46816789	-6.42036929	-0.05632861
C	-3.68161755	-5.59495851	-0.85983026
H	-6.01551468	-4.73947993	-3.19131172
H	-7.39105050	-6.25589402	-1.79032831
H	-6.40843576	-7.31777962	0.23335763
H	-4.03205053	-6.88423733	0.82436370
H	-2.63766821	-5.42684105	-0.61304883
S	-4.73955254	-1.85675383	-1.18255352
C	-4.97448692	-0.09138989	-1.45429033
C	-4.13911626	0.65727416	-2.29255400
C	-4.41492623	2.00720142	-2.51182882
C	-5.53737467	2.60245019	-1.93210129
C	-6.37846523	1.84630537	-1.11239007
C	-6.09424949	0.50369848	-0.85888137
H	-3.26665091	0.21758432	-2.76327637
H	-3.73989977	2.57766206	-3.14246451
H	-5.75334178	3.65170890	-2.11344926
H	-7.24988157	2.30412470	-0.65170182
H	-6.73090522	-0.07617125	-0.19649385
S	-2.95615219	-0.21492742	0.96224951
C	-1.88434574	-0.49879562	2.38102364
C	-1.63733249	-1.79356835	2.85892692
C	-0.86643775	-1.97339552	4.00647099
C	-0.36513806	-0.86771771	4.70035818
C	-0.63505026	0.42163213	4.23943962
C	-1.38769465	0.60942428	3.07780437
H	-2.05087438	-2.65062316	2.33577243
H	-0.66901096	-2.97817213	4.36986235
H	0.22817202	-1.01223260	5.59856663
H	-0.25086602	1.28462511	4.77588234
H	-1.58617291	1.61191507	2.70964153
Hg	4.52703445	-1.07336963	3.19952898
Cl	6.54289078	-0.93760871	-0.94012434
O	6.31560546	-0.24331341	0.37823420
O	5.26612210	-0.86173782	-1.74632741
O	6.89932077	-2.36291221	-0.71072238
O	7.62770460	-0.23030169	-1.68784462
Cl	0.07319670	1.79614596	-3.35746428
O	-0.17453778	2.44625937	-2.02676697
O	1.08068685	0.69044044	-3.18910013
O	0.60689457	2.81098134	-4.31669256
O	-1.20452754	1.21920039	-3.88466796

Compound **7**: G_{MeCN} = -5199.392952 au

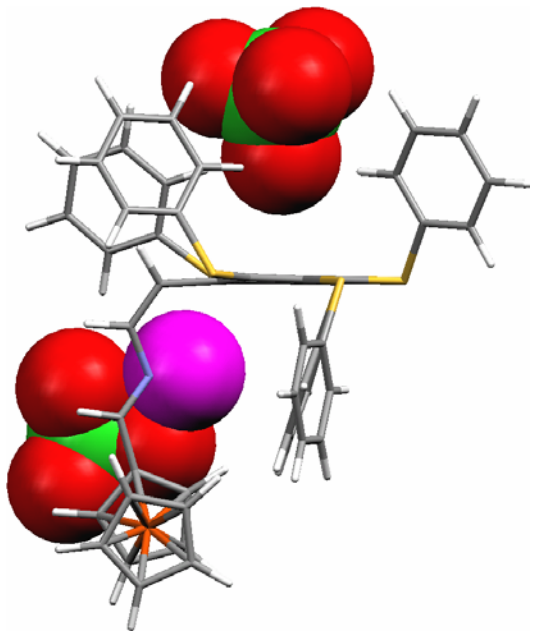
C	0.00000000	0.00000000	0.00000000
N	1.28735558	0.00000000	0.00000000
C	1.92318888	1.23387790	0.00000000
C	3.26001593	1.37668834	-0.02737121
H	-0.57111576	0.94363676	-0.02130999
H	1.29940737	2.13598556	0.01611749
H	3.66379243	2.38509465	-0.05969697
C	-0.79183232	-1.21722206	0.01832931
C	-0.31520482	-2.55997537	0.19899326
C	-1.43700718	-3.43427509	0.16503685
C	-2.61615614	-2.64712273	-0.01879100
C	-2.22488761	-1.28130349	-0.10069384

H	0.71994444	-2.83459945	0.34465905
H	-1.40733679	-4.50977497	0.28300112
H	-3.62989718	-3.02216136	-0.07220860
H	-2.88386096	-0.43359503	-0.24063323
Fe	-1.63195764	-2.06861024	1.69073840
C	-1.07967775	-0.94233739	3.31933757
C	-2.50184125	-0.96717881	3.19211538
C	-2.92505225	-2.32900749	3.26429652
C	-1.76369110	-3.14218797	3.43381708
C	-0.62188273	-2.28492822	3.46694609
H	-0.44958406	-0.06341278	3.27835728
H	-3.14529260	-0.10753685	3.05607001
H	-3.94515685	-2.68329814	3.19049249
H	-1.75050812	-4.22179427	3.50938923
H	0.40902195	-2.59908011	3.56166018
C	4.24416416	0.26314487	-0.07994930
C	4.92811212	0.02644797	-1.28963503
C	5.84631972	-1.04138419	-1.41240341
C	6.15554683	-1.82372894	-0.27532705
C	5.46353342	-1.60286241	0.94164001
C	4.53742499	-0.53949370	1.04519930
S	4.50449173	1.08798535	-2.67871926
C	6.06489684	1.87332568	-3.09064882
C	6.34073837	2.10899366	-4.44349325
C	7.49257457	2.80587414	-4.80951615
C	8.38655868	3.25258969	-3.83515560
C	8.11515633	3.00921972	-2.48707809
C	6.95365577	2.33486475	-2.11045796
H	5.66113380	1.73567326	-5.20392444
H	7.69827019	2.98396988	-5.86170366
H	9.28883201	3.78463812	-4.12342161
H	8.80328915	3.35779251	-1.72123027
H	6.73656070	2.16917261	-1.05928997
S	6.60395252	-1.36791902	-3.00788888
C	6.01240632	-3.02126499	-3.38295226
C	6.90383308	-3.91665142	-3.98676616
C	6.45935114	-5.17601481	-4.39150282
C	5.13423709	-5.55801914	-4.17733243
C	4.24863129	-4.66708876	-3.56642789
C	4.67745453	-3.39695222	-3.18099346
H	7.94208420	-3.63022336	-4.12591450
H	7.15731240	-5.86489660	-4.86001040
H	4.79325777	-6.54314496	-4.48354718
H	3.21284139	-4.95339163	-3.40310247
H	3.97866080	-2.69839468	-2.73098020
S	7.40392508	-3.11420783	-0.40756275
C	8.68703164	-2.51876845	0.69759848
C	9.10676951	-1.18180413	0.69956994
C	10.16437462	-0.78695154	1.51876872
C	10.82741698	-1.72108119	2.31795215
C	10.41874601	-3.05547167	2.30252079
C	9.34531354	-3.45456897	1.50530470
H	8.61316530	-0.45826011	0.05787349
H	10.48136068	0.25286826	1.51949597
H	11.65596607	-1.41033931	2.94836301
H	10.92425848	-3.78843044	2.92577811
H	9.00747045	-4.48657318	1.51639718
S	5.83336489	-2.63437207	2.36880509
C	4.31458461	-3.56437264	2.58590448
C	3.84903837	-3.76629876	3.89141580
C	2.74970398	-4.59617957	4.12066651
C	2.09577489	-5.20966643	3.05063548
C	2.55178153	-4.99427924	1.74677477
C	3.66291465	-4.18493898	1.51090890
H	4.34508684	-3.27112243	4.72082046
H	2.40024390	-4.75402890	5.13765681
H	1.24050350	-5.85541776	3.23033290
H	2.05467242	-5.47680281	0.90905525
H	4.03076466	-4.04472709	0.49925695
S	3.73562191	-0.20331425	2.62109328
C	4.29293417	1.46502747	2.97017251
C	3.37541844	2.36279528	3.53112156
C	3.78713349	3.64242993	3.90618701
C	5.10810762	4.04475969	3.70433317
C	6.02173991	3.15172544	3.13893186
C	5.62459049	1.86254963	2.78500296
H	2.34088047	2.05977105	3.66462795
H	3.06746077	4.33055207	4.34202158
H	5.42455364	5.04514106	3.98625792
H	7.05509047	3.45336249	2.98763782
H	6.34560631	1.16377208	2.37191633

Complex **7**·$Pb(ClO_4)_2$: G_{MeCN} = -6724.546989 au

C	0.00000000	0.00000000	0.00000000
N	1.30135318	0.00000000	0.00000000
C	1.97037686	1.23899992	0.00000000
C	3.23866910	1.41570798	0.39542206
H	-0.53339968	0.95198278	-0.09502969
H	1.38055574	2.10097284	-0.31329154
H	3.62156868	2.43153338	0.36587164
C	4.16384781	0.38231807	0.93399194
C	4.94101069	-0.43219586	0.08639013
C	5.83094282	-1.39742561	0.60889466
C	5.98859349	-1.52230121	2.00611717
C	5.17046105	-0.75034618	2.86859691
C	4.31785638	0.24483327	2.33472318
S	4.77115933	-0.36371268	-1.72017241
C	4.68971427	1.37424279	-2.19708477
C	3.74572265	1.76651206	-3.15292821
C	3.78426202	3.07814467	-3.62823927
C	4.73980588	3.97741301	-3.14568677
C	5.67277495	3.56543345	-2.19184818
C	5.66625801	2.25153863	-1.71752108
H	2.99435627	1.07211287	-3.51561889
H	3.05806229	3.39603453	-4.37143182
H	4.75752696	4.99836654	-3.51719963
H	6.42616203	4.24190728	-1.80169838
H	6.40504269	1.93782439	-0.98427628
S	6.74447358	-2.47645949	-0.50801191
C	5.43898073	-3.62587547	-0.97120701
C	4.73466957	-4.37351191	-0.01064666
C	3.75426364	-5.28595179	-0.40992402
C	3.47522135	-5.47788239	-1.76796715
C	4.18566221	-4.75068169	-2.72775724
C	5.15968622	-3.82479799	-2.33404694
H	4.97066569	-4.25476260	1.04265693
H	3.22426637	-5.86530601	0.34139949
H	2.71939839	-6.19434831	-2.07563969
H	3.98299644	-4.89859509	-3.78479030
H	5.70407846	-3.25274674	-3.07929743
S	7.19073547	-2.70000165	2.62375168
C	8.18814424	-1.72810302	3.76235661
C	8.59810675	-0.42812016	3.44614380

C	9.43446861	0.25759869	4.32952890
C	9.88819092	-0.36152503	5.49619386
C	9.49077588	-1.66797615	5.79300098
C	8.62825654	-2.35248684	4.93615700
H	8.27630399	0.05493476	2.52866467
H	9.72515106	1.27275168	4.07772577
H	10.54924840	0.17196184	6.17392914
H	9.83733528	-2.15251400	6.70226353
H	8.29162554	-3.35609609	5.18022462
S	5.23843653	-1.03546082	4.63937273
C	3.59168736	-1.66081719	4.98243725
C	2.93161283	-1.19090297	6.12569204
C	1.71746931	-1.75871871	6.51682531
C	1.14343020	-2.78450233	5.76293698
C	1.79379353	-3.24376161	4.61250558
C	3.01653152	-2.69370474	4.22732358
H	3.36970163	-0.38138792	6.70141531
H	1.21806913	-1.39314971	7.40994045
H	0.20381590	-3.23216634	6.07557393
H	1.36298028	-4.05677721	4.03253859
H	3.54008222	-3.07834457	3.35707856
S	3.35539049	1.27166649	3.45040129
C	3.84293307	2.94089037	2.99149728
C	2.84798353	3.92846285	2.99346461
C	3.19314188	5.25560115	2.73383088
C	4.51742972	5.59299780	2.44287791
C	5.50341828	4.60348132	2.43133734
C	5.17527793	3.27795124	2.72469503
H	1.81457950	3.65906944	3.19540494
H	2.42193270	6.02180957	2.74322968
H	4.77996189	6.62453975	2.22454664
H	6.53578586	4.83805305	2.19496986
H	5.96218380	2.53143284	2.73066842
C	-0.79743072	-1.19146508	0.14891068
C	-0.44248822	-2.39933095	0.86083642
C	-1.55144524	-3.28782761	0.78555139
C	-2.59150393	-2.64855878	0.04509961
C	-2.14901599	-1.35331756	-0.33042591
H	0.47147414	-2.56162406	1.41816864
H	-1.60889052	-4.26882742	1.23809680
H	-3.56263966	-3.07090361	-0.17535834
H	-2.69305216	-0.63394576	-0.92665636
Fe	-2.08842561	-1.51466900	1.69886493
C	-2.00770729	0.08446167	3.00494761
C	-3.32768592	-0.06864360	2.48290397
C	-3.79026622	-1.37176936	2.83947720
C	-2.75426349	-2.02095539	3.57674049
C	-1.65032803	-1.12119650	3.67766970
H	-1.37632165	0.95701310	2.89763015
H	-3.87987089	0.66877703	1.91526864
H	-4.75206801	-1.79686733	2.58405302
H	-2.79596869	-3.02503280	3.97823209
H	-0.70626625	-1.32070332	4.16730333
Pb	2.36605141	-1.92861518	-1.24345466
Cl	0.23472568	-1.52860709	-3.65067054
O	0.12411411	-2.70823404	-2.71133464
O	1.58997603	-0.84479597	-3.21500208
O	0.35772635	-1.95227449	-5.04738436
O	-0.85198055	-0.56181734	-3.42598567
Cl	8.51422818	2.56086035	0.90188356
O	7.65495383	1.33306519	0.65863824
O	7.91523412	3.71446905	0.15521567
O	9.89991871	2.30146743	0.44210151
O	8.49270170	2.85911050	2.37210224



Complex **7**·$Hg(ClO_4)_2$: G_{MeCN} = -6874.569025 au

C	0.00000000	0.00000000	0.00000000
N	1.30170309	0.00000000	0.00000000
C	1.94798714	1.25003126	0.00000000
C	3.20269130	1.47005544	0.42284811
H	-0.53351591	0.95677359	-0.05861686
H	1.35507643	2.09724308	-0.35085982
H	3.55220868	2.49773085	0.39088925
C	4.12443555	0.48013079	1.03537560
C	4.77445147	-0.52314060	0.29715598
C	5.57133474	-1.51304448	0.91776112
C	5.78259958	-1.45507989	2.31300980
C	5.15858149	-0.43189412	3.07135125

C	4.39130253	0.56378977	2.42336896
S	4.64315380	-0.63043762	-1.50363309
C	4.64900265	1.04073251	-2.19306027
C	3.70893105	1.40178761	-3.16397998
C	3.85194624	2.63541497	-3.79966399
C	4.91103420	3.48395375	-3.46361131
C	5.84070463	3.09866877	-2.49634132
C	5.72685975	1.86247686	-1.85626089
H	2.87439609	0.75635140	-3.42334455
H	3.12683983	2.93067880	-4.55249190
H	5.01133678	4.44431015	-3.96141636
H	6.67756656	3.73321300	-2.22411379
H	6.46849810	1.56318830	-1.12001144
S	6.35612483	-2.81736773	-0.03227868
C	4.96523734	-3.68142638	-0.74991482
C	3.69340906	-3.76107738	-0.14917226
C	2.66903943	-4.49590362	-0.76943085
C	2.90357355	-5.16765496	-1.97413241
C	4.17127364	-5.10234903	-2.55487502
C	5.19176121	-4.35887038	-1.95728061
H	3.51923455	-3.29397782	0.81624940
H	1.69522410	-4.56356290	-0.29218295
H	2.10577171	-5.72839271	-2.44972955
H	4.36830795	-5.61977465	-3.48944607
H	6.16655036	-4.29616835	-2.43286044
S	6.79726789	-2.72482424	3.07290135
C	8.08602195	-1.80022247	3.92115532
C	8.67700957	-0.66613847	3.35465012
C	9.72033846	-0.02976393	4.03063659
C	10.19379775	-0.54145140	5.24048758
C	9.61007631	-1.68636767	5.78915625
C	8.54514800	-2.31268055	5.14105234
H	8.33766026	-0.27234576	2.40194869
H	10.15274455	0.86102131	3.58590648
H	11.01376601	-0.04924147	5.75644170
H	9.97037027	-2.08576439	6.73376218
H	8.06837930	-3.18351797	5.58209964
S	5.38147933	-0.40265315	4.85248287
C	3.71434883	-0.69538603	5.45674938
C	3.18655515	0.16949778	6.42384615
C	1.95655065	-0.11698903	7.01979519
C	1.24137562	-1.25585507	6.64574063
C	1.76634843	-2.11691756	5.67643619
C	3.00251506	-1.84591028	5.08887813
H	3.73722621	1.06322597	6.69966110
H	1.55527229	0.55640567	7.77221364
H	0.28498205	-1.47718463	7.11136658
H	1.22620770	-3.01906870	5.39906327
H	3.42987938	-2.53499208	4.36652705
S	3.67074840	1.90280725	3.37926299
C	4.42926543	3.36017193	2.64364177
C	3.63676461	4.51212656	2.53751201
C	4.20068539	5.69572009	2.05835337
C	5.53915485	5.72545838	1.65940149
C	6.32140130	4.57212982	1.75538983
C	5.77627052	3.39052699	2.26277264
H	2.58981818	4.48093386	2.82781978
H	3.58650875	6.58961961	1.98406774
H	5.97124089	6.64497122	1.27407515
H	7.35992600	4.56772094	1.44169572
H	6.40948905	2.51392667	2.34644177
C	-0.81246329	-1.18416770	0.10060827
C	-0.45357298	-2.45228430	0.68451604
C	-1.58960306	-3.30367688	0.61114390
C	-2.65695058	-2.57873624	-0.00135649
C	-2.19810285	-1.26922256	-0.29809004
H	0.50171487	-2.68906349	1.13274023
H	-1.64703138	-4.31801676	0.98348370
H	-3.65303947	-2.95605469	-0.18944402
H	-2.76218346	-0.48653823	-0.78695775
Fe	-2.01610127	-1.60250434	1.70345386
C	-1.99221316	-0.02452905	3.03713869
C	-3.33359401	-0.35049622	2.67825721
C	-3.56738504	-1.71033028	3.04679709
C	-2.36929489	-2.22095063	3.63118885
C	-1.39193599	-1.18006998	3.62192468
H	-1.50458105	0.92902030	2.88080335
H	-4.04553533	0.31126081	2.20274982
H	-4.48714493	-2.26038144	2.89673074
H	-2.22412672	-3.22769416	4.00092744
H	-0.37849389	-1.24952298	3.99404646
Hg	2.32486500	-1.53991738	-1.67069152
Cl	0.02491591	-1.63542264	-3.80157863
O	0.64652710	-2.55766469	-2.64011703
O	0.56070909	-0.26214712	-3.53152149
O	0.50413600	-2.16776608	-5.08411984
O	-1.43364389	-1.70462608	-3.64486298
Cl	8.84054440	1.85764171	0.36986503
O	7.74700219	0.80094481	0.37129740
O	8.41082953	2.97979628	-0.52653259
O	10.10917895	1.25988354	-0.11016150
O	8.99180803	2.37109410	1.76960988

Calculated structures: cartesian coordinates (in Å) and energies computed for compounds **8** and their precursors**.-**

Me-CH=N-CH-P(O)$(OMe)_2^-$: G_{THF} = -819.200247 au

C	0.00000000	0.00000000	0.00000000	O	4.27911621	-0.30590843	-0.73351061
N	1.29352552	0.00000000	0.00000000	C	3.86898081	-0.46074467	-2.08266477
C	2.05134625	1.12985598	0.00000000	H	2.79563903	-0.67268978	-2.13995330
H	-0.57937911	0.94111323	0.02234469	H	4.09281107	0.43424690	-2.67999742
H	1.59959540	2.12956116	0.01578107	H	4.43256670	-1.30695299	-2.49689151
C	-0.78397409	-1.28257752	-0.03264146	O	4.28254165	0.56745211	1.55748767
H	-1.45153394	-1.40441972	0.84011427	C	5.68224764	0.46925059	1.76688545
H	-1.43439907	-1.37346981	-0.92250797	H	5.84940225	0.35908272	2.84624527
H	-0.08512009	-2.12676229	-0.04069733	H	6.10218916	-0.40670654	1.25235476
P	3.76097159	1.06797598	0.05406715	H	6.19998836	1.36875786	1.41076915
O	4.50986601	2.30400978	-0.36229617				

Ph-CH=N-CH-P(O)$(OMe)_2^-$: G_{THF} = -1011.000752 au

C	0.00000000	0.00000000	0.00000000	H	-4.04365250	-2.26178588	-0.07537466
N	1.31468215	0.00000000	0.00000000	H	-2.68498623	-0.20483856	-0.02690953
C	2.04753001	1.11554234	0.00000000	P	3.78273803	1.06137072	-0.00651406
H	-0.56253327	0.94771624	0.01767175	O	4.48482332	2.29298512	-0.49635493
H	1.59440363	2.11571690	0.00319792	O	4.26626563	-0.32323563	-0.76939083
C	-0.77380348	-1.21632621	-0.02674374	C	3.89903602	-0.47376745	-2.13587688
C	-0.17424484	-2.50382641	-0.04191568	H	4.43533888	-1.34997296	-2.51749640
C	-0.94459529	-3.65824905	-0.06907025	H	2.82018494	-0.63712627	-2.22917253
C	-2.34658949	-3.59695846	-0.08244515	H	4.18876723	0.40533102	-2.72653620
C	-2.95644317	-2.33826744	-0.06632589	O	4.30462562	0.62402293	1.49882954
C	-2.19092883	-1.17586169	-0.03898423	C	5.70901719	0.54405127	1.71388573
H	0.91029295	-2.55569370	-0.02848477	H	5.86799461	0.45742136	2.79473908
H	-0.44798708	-4.62839873	-0.07912439	H	6.13364872	-0.33826560	1.21732737
H	-2.94422897	-4.50577300	-0.10381588	H	6.21667954	1.44191980	1.34161029

$(PhS)_5$Ph-CH=N-CH-P(O)$(OMe)_2^-$: G_{THF} = -4157.524136 au

C	0.00000000	0.00000000	0.00000000	H	-4.03316916	3.11050861	0.31776915
N	1.34615639	0.00000000	0.00000000	H	-4.07882521	4.58550276	2.29912000
C	2.00776058	1.12554146	0.00000000	H	-3.08083447	3.82620556	4.45405564
H	-0.51873770	0.96018858	0.01013830	H	-2.03791552	1.56825664	4.58786131
H	1.51235354	2.10665472	-0.02410267	H	-1.99237190	0.09213063	2.60619836
C	-0.79152856	-1.15863850	0.06037965	S	-4.69978606	-1.84962564	1.20286004
C	-2.23091545	-1.03936424	0.26577738	C	-5.66894818	-2.68064356	-0.04294308
C	-2.99527284	-2.13108599	0.69440065	C	-6.98878472	-3.01966355	0.29281470
C	-2.41584014	-3.42235443	0.83826127	C	-7.82649393	-3.60682304	-0.65358502
C	-1.09776744	-3.60721628	0.33196610	C	-7.35831778	-3.87966197	-1.94092158
C	-0.31347486	-2.52674644	-0.09649141	C	-6.04312714	-3.54972108	-2.27231381
S	-3.03904777	0.50639153	-0.15815082	C	-5.20235578	-2.94581239	-1.33707691
C	-3.01177516	1.49785391	1.32964122	H	-7.35239888	-2.83004139	1.29943856
C	-3.59693727	2.77223074	1.25470669	H	-8.84634523	-3.86494025	-0.37724654
C	-3.62123925	3.60149500	2.37365227	H	-8.00935576	-4.34750937	-2.67492392
C	-3.06308169	3.17718600	3.58239329	H	-5.66434257	-3.75725464	-3.27029824
C	-2.48031473	1.91152087	3.65571966	H	-4.18568568	-2.68164741	-1.60849527
C	-2.45271967	1.07239549	2.54071205	S	-3.33687185	-4.77067527	1.55104625

C	-2.98227954	-4.67635189	3.30286711
C	-3.68641572	-5.55906993	4.13819188
C	-3.45879944	-5.56223046	5.51239351
C	-2.52972351	-4.68512768	6.07866833
C	-1.83068448	-3.80737938	5.24912563
C	-2.04979416	-3.79951924	3.87052746
H	-4.41536931	-6.24101507	3.70628366
H	-4.01401000	-6.25203500	6.14449116
H	-2.35424260	-4.68665693	7.15142613
H	-1.10237480	-3.12023543	5.67377569
H	-1.49616919	-3.11721196	3.23420408
S	-0.36663780	-5.25395665	0.33835568
C	-1.31641204	-6.14408538	-0.88241692
C	-1.42911461	-7.53433261	-0.73333386
C	-2.08317300	-8.29455659	-1.70189602
C	-2.64929121	-7.67927425	-2.82034216
C	-2.54439639	-6.29438645	-2.96498682
C	-1.87416221	-5.52847036	-2.01128166
H	-1.01294725	-8.01401155	0.14848162
H	-2.16425919	-9.37136475	-1.57161000
H	-3.16936650	-8.27172474	-3.56879245
H	-2.97826985	-5.80315164	-3.83286409
H	-1.77794329	-4.45534435	-2.14054282
S	1.14888309	-2.84307542	-1.09276062
C	2.48401281	-3.17725010	0.04253055
C	2.50733295	-2.72659050	1.36752267
C	3.59975289	-3.02048881	2.18329422
C	4.68416274	-3.74955670	1.69077295
C	4.66309847	-4.19354575	0.36671221
C	3.56749142	-3.92003506	-0.45037816
H	1.68466991	-2.13203023	1.74649002
H	3.60533885	-2.66243364	3.21010880
H	5.53335859	-3.97321052	2.33201169
H	5.49634550	-4.76967668	-0.03014071
H	3.54384450	-4.29205995	-1.47185995
P	3.78310334	1.15459909	0.01833953
O	4.38146585	2.42193393	-0.49841343
O	4.33056793	-0.19518954	-0.71785048
C	4.12534173	-0.33083236	-2.12538632
H	4.69981746	-1.20522325	-2.44240894
H	3.06505620	-0.49774362	-2.34082329
H	4.48264435	0.55647494	-2.66128734
O	4.20302576	0.77768091	1.54794248
C	5.58281947	0.54459686	1.84317216
H	5.68015647	0.56277075	2.93257077
H	5.89229204	-0.43463313	1.46382588
H	6.21698638	1.32729518	1.41103044

Fc-CH=N-CH-P(O)(OMe)$_2^-$: G_{THF} = -2429.571548 au

C	0.00000000	0.00000000	0.00000000
N	1.31226174	0.00000000	0.00000000
C	2.04969189	1.11556727	0.00000000
H	-0.57300528	0.94057980	0.02628422
H	1.59893634	2.11645339	0.01111327
C	-0.75206154	-1.23016339	-0.02103026
C	-0.23504432	-2.57062418	-0.02167739
C	-1.32151541	-3.49824950	-0.09287433
C	-2.53726693	-2.74751782	-0.07417855
C	-2.18376676	-1.36151040	0.00021398
H	0.81929614	-2.80962089	0.00404526
H	-1.23643950	-4.57777989	-0.13701843
H	-3.54288570	-3.14994273	-0.10833099
H	-2.88110341	-0.53274791	0.04368376
Fe	-1.46811077	-2.41303046	1.61963333
C	-0.32567345	-2.05023858	3.28987160
C	-1.51510132	-1.26664905	3.32525489
C	-2.63622164	-2.15499329	3.28502129
C	-2.13456017	-3.49292329	3.22826123
C	-0.70599927	-3.42739998	3.22978255
H	0.68450565	-1.66330548	3.25450851
H	-1.55626177	-0.18497670	3.33619250
H	-3.67981338	-1.86497159	3.28891015
H	-2.73144413	-4.39591625	3.18337068
H	-0.02915491	-4.27102213	3.17586535
P	3.78171825	1.05572802	-0.00568481
O	4.49050950	2.29721698	-0.46010447
O	4.26540382	-0.30979927	-0.80598797
C	3.89938669	-0.41963500	-2.17596914
H	4.43308342	-1.28623617	-2.58277529
H	2.81991836	-0.57629414	-2.27620257
H	4.19231931	0.47510452	-2.74116762
O	4.30162918	0.57215319	1.48724654
C	5.70539186	0.47720868	1.69920740
H	5.86449878	0.35868242	2.77706778
H	6.12472491	-0.39294839	1.17723446
H	6.21849219	1.38227858	1.35263752

Me-CHO (C_s): G_{THF} = -153.876544 au

C	0.00000000	0.00000000	0.00000000
H	1.11424451	0.00000000	0.00000000
C	-0.63254027	1.36924285	0.00000000
H	-1.72180332	1.28738806	-0.00000000
H	-0.29846445	1.93349842	0.88075643
H	-0.29846445	1.93349842	-0.88075643
O	-0.61436077	-1.04307559	-0.00000000

Ph-CHO (C_s): G_{THF} = -345.667136 au

C	0.00000000	0.00000000	0.00000000
H	1.11324085	0.00000000	0.00000000
O	-0.62001720	-1.04631880	-0.00000000
C	-0.61510149	1.34645147	0.00000000
C	-2.01158459	1.48638304	-0.00000000
C	-2.58109863	2.75505809	0.00000000
C	-1.76107299	3.89000892	0.00000000
C	-0.37068682	3.75660191	0.00000000
C	0.20101319	2.48502496	0.00000000
H	-2.62246393	0.58874688	-0.00000000
H	-3.66185263	2.86697140	-0.00000000
H	-2.20890118	4.88028921	0.00000000
H	0.26202770	4.63971582	0.00000000
H	1.28299653	2.36884515	0.00000000

$(PhS)_5$Ph-CHO: G_{THF} = -3492.184873 au

C	0.00000000	0.00000000	0.00000000
O	1.21216072	0.00000000	0.00000000
H	-0.57281168	0.94804779	0.00000000
C	-0.84296254	-1.25862048	0.02968040
C	-1.50748941	-1.56723579	1.22358707
C	-2.33262853	-2.70888336	1.30321084
C	-2.35810274	-3.61416758	0.21205992
C	-1.73266324	-3.26742948	-1.01341035
C	-0.97870857	-2.07449643	-1.10367268
S	-1.25671579	-0.44928478	2.62099386
C	0.37484289	-0.95342736	3.19905994
C	1.34894394	0.03327921	3.38563730
C	2.59149398	-0.31031081	3.92138766
C	2.87190187	-1.63627230	4.25151480
C	1.89985728	-2.62050552	4.05525135
C	0.64797917	-2.28371036	3.54199314
H	1.13985127	1.06026278	3.10292663
H	3.34479421	0.45978036	4.06339999
H	3.84321952	-1.90302789	4.65897772
H	2.11028642	-3.65470610	4.31498746
H	-0.11230893	-3.04747217	3.41240146
S	-3.29542622	-3.05516904	2.78096671
C	-4.35782970	-1.61081285	2.88976261
C	-4.58312057	-1.05504599	4.15507706
C	-5.48861758	-0.00382083	4.30234724
C	-6.15525205	0.51275702	3.19020942
C	-5.92339742	-0.03790117	1.92777305
C	-5.03988107	-1.10631531	1.77493549
H	-4.04113889	-1.43699249	5.01501084
H	-5.65865346	0.42227260	5.28748979
H	-6.85109935	1.33908220	3.30562500
H	-6.44384093	0.35454943	1.05803354
H	-4.88371035	-1.55016286	0.79647574
S	-3.20720870	-5.19085355	0.34890073
C	-2.34980648	-5.96883713	1.72258574
C	-0.95156961	-5.96960702	1.82057395
C	-0.32948994	-6.66286419	2.85899861
C	-1.08981923	-7.38026822	3.78581309
C	-2.48098872	-7.39220602	3.67633931
C	-3.11351419	-6.68065839	2.65590217
H	-0.35522062	-5.43676855	1.08635326
H	0.75507070	-6.65676084	2.93092823
H	-0.60028461	-7.92651747	4.58726054
H	-3.08063419	-7.94301385	4.39606244
H	-4.19720782	-6.66511796	2.58785437
S	-1.82389156	-4.33685172	-2.44928959
C	-3.58435893	-4.41794630	-2.79288040
C	-4.12222645	-5.65230670	-3.17787989
C	-5.46211325	-5.73993591	-3.55722724
C	-6.27682977	-4.60695795	-3.53365110
C	-5.74095619	-3.37837202	-3.14119445
C	-4.39629773	-3.27617889	-2.78512372
H	-3.49560492	-6.53917911	-3.16735928
H	-5.87213471	-6.70111442	-3.85557844
H	-7.32268602	-4.68012083	-3.81844002
H	-6.36728254	-2.49021818	-3.12664474
H	-3.97633675	-2.31401086	-2.50817271
S	-0.28448847	-1.47557846	-2.65432879
C	1.17148982	-2.51159674	-2.89169033
C	1.29236791	-3.22375248	-4.09049293
C	2.44595436	-3.96971335	-4.33978910
C	3.46654548	-4.02136632	-3.38949235
C	3.33856990	-3.31279426	-2.19213016
C	2.20024524	-2.54612681	-1.94134949
H	0.48415128	-3.19891708	-4.81465873
H	2.53855411	-4.52005652	-5.27234644
H	4.35983229	-4.60977917	-3.58145327
H	4.13511011	-3.34324081	-1.45323795
H	2.11224330	-1.96553744	-1.02825840

Fc-CHO: G_{THF} = -1764.248629 au

C	0.00000000	0.00000000	0.00000000
C	1.43645125	0.00000000	0.00000000
C	1.87340455	1.35229918	0.00000000
C	0.72029721	2.19825295	-0.01477459
C	-0.43614612	1.37088182	-0.02025424
H	2.05588284	-0.88604200	0.00324980
H	2.90262834	1.68710251	-0.01012385
H	0.72774236	3.28028714	-0.03469509
H	-1.46537931	1.70689026	-0.03193174
Fe	0.71586730	0.95752710	-1.65984811
C	-0.05232438	0.02594221	-3.32536006
C	-0.38001640	1.41495610	-3.33914018
C	0.84098303	2.15477290	-3.32265622
C	1.92140547	1.22211064	-3.29797756
C	1.36922574	-0.09468345	-3.29802673
H	-0.75664527	-0.79576583	-3.31340939

H	-1.37796540	1.83351533	-3.35032921	C	-0.86457494	-1.18302999	-0.04976690
H	0.93160067	3.23325038	-3.31705542	O	-0.46640276	-2.33451163	-0.04895434
H	2.97444341	1.47040832	-3.26916766	H	-1.95501356	-0.95963750	-0.08669954
H	1.92720509	-1.02114492	-3.26619364				

Compound **8a**^{erytro}: G_{THF} = -973.087559 au

C	0.00000000	0.00000000	0.00000000	H	3.97434405	-0.59370870	-0.51267194
N	1.26980070	0.00000000	0.00000000	O	3.93326663	2.13403701	-0.55330641
C	1.95886270	1.25927899	0.00000000	P	2.50137321	2.11652720	-1.64023320
C	3.42710007	1.27019987	0.44551173	O	2.44122489	3.58825158	-1.97997582
H	-0.58566614	0.93372804	0.02213027	O	0.92601906	1.60118519	-2.34073354
H	1.38349740	2.04667953	0.51684791	C	0.19127375	2.44613633	-3.17886235
H	3.55386515	1.72893464	1.44489684	H	-0.88781266	2.29307894	-2.99546917
C	-0.79044713	-1.27670408	-0.07331302	H	0.44036876	3.49992598	-3.00678697
H	-1.51320867	-1.35367512	0.75249333	H	0.36616307	2.23081694	-4.25288811
H	-1.36911541	-1.31725743	-1.00752590	O	3.36699950	1.09414708	-2.65182458
H	-0.11362861	-2.13546967	-0.04236577	C	2.90904602	0.82014482	-3.96140378
C	4.11878932	-0.09517103	0.44970476	H	3.71295139	0.26696058	-4.46567556
H	5.19515703	0.04917803	0.60770668	H	1.99427769	0.21762708	-3.95929310
H	3.72626672	-0.74632948	1.24205934	H	2.71795570	1.74140044	-4.52943984

Compound **8a**^{threo}: G_{THF} = -973.090804 au

C	0.00000000	0.00000000	0.00000000	H	3.19178671	1.10280647	2.66695092
N	1.26988679	0.00000000	0.00000000	O	3.95656963	2.12506809	-0.46711673
C	1.95812391	1.26020741	0.00000000	P	2.58780109	2.05644436	-1.63572852
C	3.40224799	1.25628045	0.49885413	O	2.57022619	3.50901624	-2.05354593
H	-0.58648777	0.93379838	0.02344913	O	1.04766288	1.52756643	-2.39484381
H	1.36973503	2.06173468	0.48239724	C	0.39197206	2.32368203	-3.34000070
H	3.80347250	0.22828289	0.41741794	H	-0.69987549	2.19757152	-3.22619991
C	-0.79111928	-1.27639649	-0.07306032	H	0.64738501	3.38309663	-3.21984479
H	-1.51143644	-1.35454066	0.75477451	H	0.64009235	2.03393947	-4.38152241
H	-1.37239315	-1.31633643	-1.00568661	O	3.50110118	0.96908871	-2.52600891
H	-0.11405275	-2.13502991	-0.04497581	C	3.10163469	0.56782994	-3.82097444
C	3.64059791	1.77080832	1.91809799	H	3.91917877	-0.04424154	-4.22559579
H	4.71593873	1.84427187	2.12389604	H	2.17764952	-0.01985522	-3.80345267
H	3.20819341	2.77249638	2.03378444	H	2.95449566	1.42752744	-4.49013539

Compound **8b**^{erytro}: G_{THF} = -1356.655392 au

C	0.00000000	0.00000000	0.00000000	H	-0.39101105	-4.63681107	-0.16107557
N	1.27533020	0.00000000	0.00000000	H	-2.87847684	-4.53676908	-0.11862816
C	1.97421609	1.24038043	0.00000000	H	-4.02077620	-2.32680371	-0.03165349
C	3.44493668	1.22272566	0.47868930	H	-2.67905901	-0.23903708	0.01400934
H	-0.58759488	0.93094127	0.02529235	C	4.01077385	-0.13959471	0.85173509
H	1.39476653	2.05239151	0.47080592	C	4.65004542	-0.93139962	-0.10971938
H	3.56149509	1.87906500	1.36224428	C	5.17487380	-2.17775633	0.23527082
C	-0.77819842	-1.24944483	-0.04312479	C	5.07524720	-2.65255253	1.54599970
C	-0.14319442	-2.50381836	-0.09485605	C	4.44470733	-1.86574140	2.51248764
C	-0.89508991	-3.67357884	-0.12053574	C	3.92224047	-0.61923340	2.16411328
C	-2.29432729	-3.61938866	-0.09676839	H	4.72188215	-0.54478356	-1.12109059
C	-2.93422016	-2.38005714	-0.04754593	H	5.66833484	-2.78300907	-0.52338124
C	-2.18052618	-1.20591443	-0.02032623	H	5.48918613	-3.62312442	1.81322330
H	0.94196448	-2.52394732	-0.11421603	H	4.36549447	-2.22024135	3.53886609

H	3.43779806	-0.00588403	2.92296743
O	4.05359775	1.79034366	-0.65533270
P	2.58425869	1.97567187	-1.68765242
O	2.68902233	3.44784172	-2.00563064
O	0.95203029	1.63896291	-2.32065531
C	0.27768658	2.56897748	-3.12422718
H	-0.80424370	2.49969583	-2.91904348
H	0.62025503	3.59182480	-2.93051953
H	0.41563924	2.36665847	-4.20437064
O	3.29756455	0.86979385	-2.72399740
C	2.76688573	0.64222530	-4.01757831
H	3.48764302	0.00138657	-4.54129004
H	1.79308643	0.14425202	-3.97634108
H	2.66084413	1.57693473	-4.58488629

Compound **8b**^{threo}: G_{THF} = -1356.662259 au

C	0.00000000	0.00000000	0.00000000
N	1.27634827	0.00000000	0.00000000
C	1.97148592	1.24346388	0.00000000
C	3.42737487	1.21530918	0.48809817
H	-0.58625932	0.93145754	0.02449858
H	1.39956770	2.05381986	0.48245677
H	3.80051182	0.17783876	0.39934932
C	-0.78256683	-1.24647430	-0.04067271
C	-0.15575110	-2.50273147	-0.12847183
C	-0.91181844	-3.66976804	-0.15159360
C	-2.30958089	-3.61099805	-0.08947873
C	-2.94249860	-2.36991057	-0.00550436
C	-2.18392309	-1.19900287	0.01855649
H	0.92814747	-2.52628856	-0.18092611
H	-0.41302418	-4.63412769	-0.22178999
H	-2.89780519	-4.52570056	-0.10977225
H	-4.02793486	-2.31280084	0.04009981
H	-2.67776375	-0.23121917	0.08071652
C	3.64858503	1.68651771	1.91357416
C	4.07992326	2.99287324	2.17267132
C	4.25603336	3.43516764	3.48534879
C	4.00366939	2.57952372	4.56039509
C	3.57427707	1.27305920	4.31030716
C	3.40236742	0.83213848	2.99774833
H	4.27723642	3.63621178	1.32101282
H	4.59499081	4.45302004	3.67058734
H	4.14315853	2.92454246	5.58312590
H	3.37620074	0.59624735	5.13968892
H	3.06870386	-0.18589064	2.80425815
O	3.98664744	2.07679117	-0.47121732
P	2.60877938	2.03431915	-1.65066162
O	2.63087762	3.48810351	-2.05695622
O	1.06637918	1.54132884	-2.38325208
C	0.41461108	2.35459384	-3.32204513
H	-0.67270986	2.19082672	-3.23652220
H	0.63852198	3.41485819	-3.15982023
H	0.69975272	2.10622241	-4.36265903
O	3.50200623	0.92660335	-2.52532220
C	3.09553314	0.51838686	-3.81844216
H	3.89923234	-0.11780155	-4.21088895
H	2.15807926	-0.04648528	-3.79440909
H	2.97213902	1.37401130	-4.49678040

Compound **8c**^{erytro}: G_{THF} = -2775.233205 au

C	0.00000000	0.00000000	0.00000000
N	1.27538785	0.00000000	0.00000000
C	1.97268522	1.24211478	0.00000000
C	3.44635505	1.23272617	0.45574287
H	-0.58645127	0.93141569	0.02319805
H	1.40422981	2.04285965	0.50241644
H	3.56858922	1.79409444	1.40053828
C	-0.78170411	-1.24748567	-0.04025107
C	-0.15321379	-2.50419649	-0.10800005
C	-0.91051713	-3.67060702	-0.13118010
C	-2.30896139	-3.61045727	-0.08879797
C	-2.94270227	-2.36867871	-0.02424704
C	-2.18350141	-1.19810835	0.00002128
H	0.93138943	-2.53008380	-0.14357412
H	-0.41131707	-4.63572679	-0.18469241
H	-2.89736166	-4.52511557	-0.10875057
H	-4.02866464	-2.31076769	0.00582041
H	-2.67730750	-0.22933850	0.04621566
C	4.05829500	-0.13236590	0.66039678
C	4.52766451	-1.01047388	-0.36129888
C	5.05728330	-2.18341247	0.25604825
C	4.92086528	-2.03789778	1.67208136
C	4.30288363	-0.77263570	1.91615195
H	4.49581979	-0.77775651	-1.41664996
H	5.50516357	-3.02720314	-0.25531385
H	5.23725790	-2.75153774	2.42346677
H	4.07550926	-0.35287101	2.88905085
Fe	6.06757534	-0.52186694	0.90752132
C	7.01985891	1.21995029	0.40218024
C	7.12030367	0.98879681	1.80764281
C	7.78042909	-0.26358180	2.01106300
C	8.09233570	-0.80728446	0.72627523
C	7.62207471	0.11019456	-0.26443724
H	6.47853132	2.02661011	-0.07496805
H	6.73304245	1.63608911	2.58442607
H	7.99958028	-0.72251680	2.96740030
H	8.58745263	-1.75204846	0.53776511
H	7.67494179	-0.02636479	-1.33691851
O	4.00549588	1.94540125	-0.62666992
P	2.52629039	2.05454577	-1.67130291
O	2.56323419	3.53311084	-1.97238684
O	0.91795456	1.64839665	-2.30963762
C	0.19775510	2.55521033	-3.10136462
H	-0.87905040	2.42385899	-2.90167778
H	0.48485445	3.59105599	-2.88868190
H	0.35116753	2.37814039	-4.18336257
O	3.30106910	0.99859865	-2.71775222
C	2.78683893	0.76977651	-4.01884655
H	3.53959169	0.17446534	-4.55078585
H	1.83780316	0.22514795	-3.99153129
H	2.63889081	1.70925001	-4.56818586

Compound **8c**^{threo}: G_{THF} = -2775.238533 au

C	0.00000000	0.00000000	0.00000000
N	1.27597689	0.00000000	0.00000000
C	1.97078749	1.24439689	0.00000000
C	3.41837076	1.21241326	0.50745249
H	-0.58629789	0.93157826	0.02619883
H	1.39127989	2.05901743	0.46584999
H	3.78153653	0.16946186	0.46565784
C	-0.78302503	-1.24630945	-0.04170086
C	-0.15647812	-2.50263473	-0.12919933
C	-0.91299236	-3.66935744	-0.15401439
C	-2.31079055	-3.60998883	-0.09388794
C	-2.94338965	-2.36875646	-0.01009795
C	-2.18434555	-1.19816777	0.01567904
H	0.92747475	-2.52672582	-0.17986996
H	-0.41451131	-4.63388131	-0.22384332
H	-2.89933278	-4.52444122	-0.11548376
H	-4.02884768	-2.31126728	0.03404203
H	-2.67791144	-0.23023118	0.07772107
C	3.63998282	1.74835288	1.89731459
C	3.78355150	0.99162599	3.10349832
C	3.98548490	1.89795537	4.19065922
C	3.96342009	3.22480060	3.65810670
C	3.75077332	3.12884655	2.24889289
H	3.76521444	-0.08948455	3.16923681
H	4.13704923	1.62724887	5.22868771
H	4.10484545	4.13883678	4.22226571
H	3.72355138	3.94078210	1.53478439
Fe	5.45781127	2.12740978	2.78272194
C	6.81666335	2.00188291	1.25642771
C	7.03127911	3.19050783	2.01821119
C	7.30229081	2.81414774	3.37057883
C	7.25590988	1.38748545	3.44655910
C	6.95813641	0.88901981	2.13958034
H	6.48659476	1.96069645	0.22611165
H	6.96144507	4.20214563	1.63941198
H	7.49766853	3.48979604	4.19429973
H	7.41100953	0.79152507	4.33753886
H	6.82592358	-0.15139675	1.87100090
O	4.00441756	2.03545336	-0.47694140
P	2.62032794	2.00362711	-1.65934874
O	2.66237515	3.45615597	-2.06849988
O	1.07715198	1.52483345	-2.39141481
C	0.43720714	2.33939136	-3.33787812
H	-0.65213201	2.19229753	-3.25058282
H	0.67686176	3.39750617	-3.18486701
H	0.71884782	2.07681172	-4.37572670
O	3.50451601	0.88177962	-2.52460179
C	3.09662168	0.46814406	-3.81610115
H	3.89371383	-0.18072897	-4.20082547
H	2.15247497	-0.08516442	-3.78988271
H	2.98564090	1.31982177	-4.50140448

Compound **8d**^{erytro}: G_{THF} = -2775.231805 au

C	0.00000000	0.00000000	0.00000000
N	1.27432947	0.00000000	0.00000000
C	1.97096832	1.24519113	0.00000000
C	3.39790464	1.22637710	0.60350392
H	-0.59062392	0.92998048	0.02221581
H	1.35208474	2.07973831	0.37177046
H	3.48336447	2.02643211	1.36456196
C	-0.76264429	-1.25185375	-0.04606066
C	-0.21969208	-2.57539955	-0.10295535
C	-1.29968706	-3.50499777	-0.11227836
C	-2.52201897	-2.76631936	-0.04353488
C	-2.18971041	-1.37922743	0.00093993
H	0.83843157	-2.79545292	-0.12690944
H	-1.21009885	-4.58381589	-0.14368179
H	-3.52075071	-3.18433225	-0.01988593
H	-2.89081652	-0.55592527	0.06292368
Fe	-1.35587938	-2.37013306	1.59384608
C	-1.09022239	-1.23321611	3.28108710
C	-2.35637937	-1.89396958	3.32108511
C	-2.11960636	-3.30155653	3.25495529
C	-0.70741509	-3.50572349	3.17418518
C	-0.07087228	-2.22758783	3.18806816
H	-0.92817836	-0.16314667	3.28304726
H	-3.32469545	-1.41258322	3.37634969
H	-2.87719521	-4.07534116	3.25221902
H	-0.20695136	-4.46205860	3.09006767
H	0.99151295	-2.03966106	3.09751376
C	3.82830918	-0.07516055	1.26085785
C	4.43697498	-1.08298337	0.50281263
C	4.82545228	-2.28241532	1.09992251
C	4.61807712	-2.49577464	2.46610834
C	4.02107159	-1.49193636	3.23249849
C	3.63500936	-0.29125461	2.63043908
H	4.59534358	-0.89607497	-0.55447820
H	5.29620677	-3.05704055	0.49699664
H	4.92692157	-3.43012088	2.93089923
H	3.86841201	-1.63763898	4.30060241
H	3.18170223	0.49408062	3.23429746
O	4.13697218	1.53187151	-0.55203285
P	2.74419615	1.80186862	-1.67735950
O	2.99366853	3.24212676	-2.05501051
O	1.12520175	1.56452855	-2.39185583
C	0.58061413	2.49890969	-3.28346572
H	-0.51109695	2.54720473	-3.12979712
H	1.01224498	3.49555857	-3.13548333
H	0.74517783	2.21385278	-4.34125250
O	3.41606811	0.58584625	-2.61034874
C	2.94516035	0.33706383	-3.92273978
H	3.63794625	-0.38765984	-4.36936624
H	1.93139016	-0.07561120	-3.92001312
H	2.95338014	1.24627646	-4.53938758

Compound **8d**^{threo}: G_{THF} = -2775.238996 au

C	0.00000000	0.00000000	0.00000000	H	0.72400044	-3.38404858	3.17315011
N	1.27565173	0.00000000	0.00000000	C	3.55320093	1.69571632	1.97904392
C	1.96300590	1.25089737	0.00000000	C	3.83764425	3.03350435	2.27972040
C	3.40198395	1.24563739	0.53873138	C	3.93220217	3.45861891	3.60597777
H	-0.58905661	0.93041488	0.00792700	C	3.74509137	2.55452287	4.65498061
H	1.37224960	2.05919332	0.46404793	C	3.46709844	1.21621321	4.36460860
H	3.80335386	0.21909562	0.44549742	C	3.37706943	0.79270519	3.03734903
C	-0.77205397	-1.24646399	-0.01905409	H	3.98997910	3.71524475	1.44870337
C	-0.24943562	-2.57951421	-0.04600707	H	4.15706060	4.50141204	3.82323082
C	-1.34279510	-3.49367331	-0.03663488	H	3.82104939	2.88703622	5.68838983
C	-2.55402156	-2.73545017	0.01273006	H	3.32689061	0.50054336	5.17278884
C	-2.20112901	-1.35314547	0.02679371	H	3.17359062	-0.25300384	2.81207966
H	0.80414476	-2.81943137	-0.07169979	O	3.96830609	2.13920898	-0.38556235
H	-1.26967918	-4.57411410	-0.04719401	P	2.63802515	2.04557831	-1.62394806
H	-3.55901756	-3.13757223	0.04195990	O	2.63512614	3.49668302	-2.04038721
H	-2.88927456	-0.51780310	0.06760031	O	1.14135406	1.50217136	-2.41553789
Fe	-1.38613823	-2.31912278	1.64369833	C	0.51171279	2.28232720	-3.39656844
C	-0.45659715	-1.48419608	3.27263574	H	-0.57567061	2.10438936	-3.34669645
C	-1.86514361	-1.25881773	3.33505900	H	0.71407477	3.34944221	-3.25142573
C	-2.51866529	-2.52937798	3.34300840	H	0.83779628	2.01347238	-4.42001781
C	-1.51206687	-3.54175638	3.28549067	O	3.60111599	0.95926215	-2.45047080
C	-0.23860437	-2.89416344	3.24260614	C	3.25894456	0.52249003	-3.75269257
H	0.30922087	-0.72138929	3.21243846	H	4.09507146	-0.09613500	-4.10332781
H	-2.35201584	-0.29221900	3.35274605	H	2.33708489	-0.06797391	-3.75832870
H	-3.58807234	-2.69610351	3.37371606	H	3.13987825	1.36518137	-4.44785632
H	-1.68418722	-4.61056672	3.26507966				

Compound **8e**^{erytro}: G_{THF} = -4503.163201 au

C	0.00000000	0.00000000	0.00000000	C	-5.81449377	-0.12493315	2.69433894
N	1.27317523	0.00000000	0.00000000	C	-6.65924451	0.91598971	2.30992270
C	2.04640285	1.22352151	0.00000000	C	-6.82049916	1.23177690	0.95978803
C	3.26479538	1.31163495	-0.97504911	C	-6.13870116	0.48925527	-0.00630131
H	-0.57235550	0.93261471	-0.00129711	C	-5.31144473	-0.56958209	0.36758772
H	2.44087993	1.30385475	1.02402157	H	-5.66313707	-0.34726305	3.74676748
H	4.20185445	1.10477812	-0.42735950	H	-7.17518728	1.49530106	3.07161028
C	-0.81804390	-1.25234008	0.11072844	H	-7.46576079	2.05419843	0.66291219
C	-1.87401231	-1.24544600	1.05751471	H	-6.25519395	0.72822729	-1.06032222
C	-2.79401949	-2.31441441	1.13090492	H	-4.79831005	-1.15383634	-0.38963217
C	-2.59295409	-3.46503115	0.33392916	S	-3.68567090	-4.88596700	0.48168652
C	-1.53579821	-3.48674895	-0.60626661	C	-3.33779802	-5.48510373	2.13393732
C	-0.64478193	-2.39031570	-0.71224528	C	-2.06023400	-5.43381128	2.70804168
S	-2.04916962	0.15772967	2.18062015	C	-1.84214711	-5.98609701	3.97034624
C	-0.56940497	0.01322369	3.20095504	C	-2.88150303	-6.61290350	4.66101730
C	0.39759982	1.02355640	3.15489917	C	-4.15082799	-6.67420359	4.08307252
C	1.48636153	0.97170842	4.03012070	C	-4.38401457	-6.10514328	2.83125382
C	1.62029624	-0.08611818	4.93031033	H	-1.24183255	-4.96536386	2.17077762
C	0.65763498	-1.09902730	4.96355048	H	-0.84854766	-5.93465465	4.40842384
C	-0.44344727	-1.04693805	4.10909900	H	-2.70435014	-7.04607765	5.64187890
H	0.31703415	1.81287579	2.41186788	H	-4.97063165	-7.15116167	4.61480453
H	2.23640639	1.75729682	3.99034488	H	-5.37940054	-6.12858918	2.39639368
H	2.47350240	-0.12459665	5.60345143	S	-1.28812141	-4.93298077	-1.64894037
H	0.75736086	-1.92533331	5.66363775	C	-2.73211367	-4.91793228	-2.70645201
H	-1.20561420	-1.81995136	4.14509175	C	-3.25636708	-6.15306447	-3.11305978
S	-4.17536703	-2.27911717	2.28291432	C	-4.31924521	-6.20060633	-4.01487776
C	-5.13876829	-0.87619356	1.72352544	C	-4.88396158	-5.02103605	-4.50350045

C	-4.36783896	-3.79056810	-4.09136940	C	3.37785266	-1.16942699	-4.52942101
C	-3.29025137	-3.73373541	-3.20758136	C	4.05692615	-1.56270989	-3.37461376
H	-2.83716336	-7.07155488	-2.71189642	C	4.00281372	-0.76612399	-2.22916955
H	-4.71734337	-7.16470604	-4.32213592	H	2.05754186	1.75776306	-3.36813719
H	-5.71948712	-5.05964852	-5.19743823	H	2.12769828	0.34358966	-5.42352411
H	-4.79550623	-2.86545191	-4.46979665	H	3.42058560	-1.78336371	-5.42698360
H	-2.87845621	-2.77419502	-2.91129739	H	4.63038530	-2.48715832	-3.36431160
S	0.66083804	-2.41248722	-1.95740250	H	4.54037985	-1.07443829	-1.33447476
C	1.85966929	-3.49953511	-1.17219603	O	3.15204415	2.67771191	-1.27576169
C	2.28723036	-4.64453424	-1.85545028	P	1.60874007	3.05276944	-0.44239751
C	3.26796051	-5.46633195	-1.29544096	O	2.03816716	4.31327080	0.26896662
C	3.80980322	-5.16135567	-0.04599027	O	0.00501429	2.83210584	0.40881245
C	3.38030510	-4.01838655	0.63434514	C	-0.63387086	3.91577944	1.04702979
C	2.41859096	-3.17822530	0.07253592	H	-1.10330557	3.56177668	1.97924334
H	1.84576304	-4.88904707	-2.81641587	H	0.08834235	4.70441727	1.28263398
H	3.59737589	-6.35269388	-1.83271788	H	-1.43779004	4.34553518	0.42357676
H	4.56595251	-5.80745493	0.39374952	O	0.88774644	3.18705550	-1.95028598
H	3.80994224	-3.76665127	1.60116882	C	-0.36786145	3.81705984	-2.12047989
H	2.12044475	-2.25507023	0.56097586	H	-0.52734061	3.91244102	-3.20147280
C	3.26916270	0.42541722	-2.21086188	H	-1.18419808	3.23088874	-1.68386990
C	2.60189586	0.81959168	-3.37869003	H	-0.38023332	4.82182775	-1.67862885
C	2.65226365	0.02519557	-4.52440984				

Compound **8e**^{threo}: G_{THF} = -4503.167467 au

C	0.00000000	0.00000000	0.00000000	C	-2.13068303	-5.49652875	2.37791297
N	1.27445122	0.00000000	0.00000000	C	-2.01619476	-6.03957636	3.65761148
C	1.96298396	1.25185164	0.00000000	C	-3.10171229	-6.68388304	4.25526396
C	3.49250014	1.22156458	0.13441332	C	-4.31230558	-6.77242505	3.56597569
H	-0.58494327	0.92355495	0.02383506	C	-4.44295505	-6.21233626	2.29507540
H	1.52813891	1.95439033	0.72699421	H	-1.27640451	-5.01587796	1.91177773
H	3.86316665	0.25365681	-0.24899930	H	-1.06716620	-5.96841524	4.18306441
C	-0.81424413	-1.24289073	-0.02142636	H	-3.00523014	-7.10994389	5.25035797
C	-1.96063857	-1.29419641	0.81404797	H	-5.16711647	-7.26365196	4.02448330
C	-2.84995658	-2.38899054	0.76341493	H	-5.39437870	-6.25664181	1.77244336
C	-2.52042036	-3.51781745	-0.02313175	S	-0.97490951	-4.89194075	-1.89732177
C	-1.38327200	-3.47580992	-0.86493261	C	-2.31244895	-4.92425672	-3.08686263
C	-0.54055516	-2.33790894	-0.87963778	C	-2.76094758	-6.17465420	-3.53465497
S	-2.30011521	0.06457126	1.95459614	C	-3.73168844	-6.25394596	-4.53318439
C	-0.85695653	0.01635349	3.02744154	C	-4.27950716	-5.09157262	-5.07876618
C	-0.11093964	1.18475747	3.21765366	C	-3.83911372	-3.84592762	-4.62599417
C	0.97155193	1.18525449	4.09894953	C	-2.85227372	-3.75689363	-3.64434988
C	1.31358976	0.02175026	4.78843202	H	-2.35629515	-7.07983221	-3.09069831
C	0.56292386	-1.14192937	4.60457916	H	-4.07208724	-7.22939482	-4.87226990
C	-0.52639342	-1.14716545	3.73428415	H	-5.04385802	-5.15512185	-5.84877157
H	-0.36063273	2.08097531	2.65772201	H	-4.25393253	-2.93411385	-5.04834454
H	1.57313527	2.08197615	4.21360052	H	-2.49536147	-2.78580946	-3.31622777
H	2.17431097	0.02076057	5.45058577	S	0.78392986	-2.21849574	-2.10197351
H	0.82472797	-2.05073149	5.14134877	C	2.07120054	-3.26126339	-1.40728378
H	-1.11576073	-2.04883733	3.59630473	C	2.61589312	-4.27197801	-2.20992397
S	-4.35601987	-2.41476565	1.74534275	C	3.67206164	-5.05022385	-1.73245312
C	-5.27282763	-1.00629046	1.12325759	C	4.17196541	-4.84199147	-0.44624141
C	-6.08352367	-0.31088703	2.03058843	C	3.62334228	-3.83654151	0.35423244
C	-6.89644316	0.73121844	1.58541567	C	2.58625119	-3.03472840	-0.12333986
C	-6.89192660	1.10431291	0.24022793	H	2.20447025	-4.44928673	-3.19892755
C	-6.07595865	0.41776184	-0.66112329	H	4.09310979	-5.82953615	-2.36340907
C	-5.27903136	-0.64249429	-0.22964162	H	4.98761722	-5.45547538	-0.07113951
H	-6.06290988	-0.57809072	3.08334846	H	4.01845860	-3.65957312	1.35193696
H	-7.51913610	1.26595537	2.29839859	H	2.19511196	-2.20921528	0.46268115
H	-7.51334046	1.92742656	-0.10207559	C	4.04577705	1.44030704	1.52964816
H	-6.06246739	0.70160055	-1.71025732	C	4.40935296	0.36277575	2.34632367
H	-4.66056183	-1.18256767	-0.93937352	C	4.88468493	0.57194443	3.64300858
S	-3.55470742	-4.98751982	0.01045536	C	5.00588090	1.87010240	4.14402065
C	-3.35050079	-5.57437333	1.69164157	C	4.65423669	2.95365325	3.33190389

C	4.18390845	2.74090578	2.03567237
H	4.32373723	-0.64943254	1.95553815
H	5.16928012	-0.27907965	4.25928155
H	5.38393155	2.03729940	5.15068625
H	4.76112761	3.96974254	3.70746919
H	3.93425269	3.56997050	1.38011781
O	3.77824119	2.29708527	-0.72657576
P	2.18475758	2.36501636	-1.58090127
O	2.05375543	3.86539109	-1.67827640
O	0.54198285	1.88689639	-2.06312093
C	-0.33406683	2.80210609	-2.66969064
H	-1.36671801	2.55486866	-2.37230555
H	-0.10501345	3.83133530	-2.37307315
H	-0.29015828	2.74878112	-3.77378460
O	2.90787416	1.51854938	-2.82114579
C	2.25518826	1.33588845	-4.06541923
H	2.98640575	0.86157017	-4.73153850
H	1.37282416	0.69503871	-3.97382616
H	1.95319899	2.29361687	-4.51096938

Compound **8f**^{erytro}: G_{THF} = -4503.161506 au

C	0.00000000	0.00000000	0.00000000
N	1.27800280	0.00000000	0.00000000
C	1.94534796	1.26803497	0.00000000
C	3.45376851	1.40164224	0.35857672
H	-0.56951641	0.93883623	0.00157241
H	1.41359388	2.00228116	0.62410291
H	3.59206542	1.67174669	1.41819112
C	-0.81428908	-1.22548824	-0.01285033
C	-0.24049179	-2.50712438	-0.05449545
C	-1.04647900	-3.64155853	-0.05571052
C	-2.43988939	-3.51804248	-0.01322816
C	-3.02179790	-2.24963140	0.02761865
C	-2.21329552	-1.11330428	0.02697323
H	0.83907083	-2.59456528	-0.08941233
H	-0.58453770	-4.62440284	-0.09712199
H	-3.06727241	-4.40658989	-0.01513360
H	-4.10404724	-2.14504658	0.05775564
H	-2.66416794	-0.12328934	0.05366265
C	4.33354505	0.17935828	0.05648743
C	4.08730546	-1.08028809	0.63634243
C	4.75189543	-2.24075103	0.17273820
C	5.67429054	-2.12902345	-0.89226215
C	5.99086742	-0.85399594	-1.41431352
C	5.43143941	0.30489215	-0.82440531
S	2.94214975	-1.16534299	2.03239549
C	4.05534917	-1.44089972	3.41290926
C	3.52392194	-2.10309282	4.53044923
C	4.29233527	-2.27672172	5.68066554
C	5.60761322	-1.81008595	5.72907748
C	6.14212500	-1.15893950	4.61588514
C	5.37271954	-0.96524216	3.46829803
H	2.50911558	-2.49010460	4.48903600
H	3.86457806	-2.79346160	6.53683987
H	6.21012588	-1.95559365	6.62203409
H	7.16444317	-0.78892746	4.63978728
H	5.79403977	-0.44372083	2.61478349
S	4.47636019	-3.82054903	0.98362986
C	3.39572272	-4.71582966	-0.12294566
C	3.10533640	-6.04120680	0.23892305
C	2.26865822	-6.82012066	-0.55730093
C	1.71191430	-6.29335929	-1.72612918
C	2.00045554	-4.97567494	-2.08381607
C	2.83486418	-4.18496664	-1.29077940
H	3.53944364	-6.46053540	1.14348421
H	2.05521840	-7.84552495	-0.26366457
H	1.06313233	-6.90292689	-2.34969718
H	1.57381996	-4.54759190	-2.98700934
H	3.04179827	-3.16081921	-1.58227431
S	6.36955536	-3.61540829	-1.63876295
C	7.76542298	-4.00323415	-0.58934229
C	8.54981412	-3.03241553	0.04605221
C	9.66496792	-3.41636121	0.79096842
C	10.02305399	-4.76165238	0.89771037
C	9.24684629	-5.72848174	0.25541280
C	8.11988551	-5.35590747	-0.47627302
H	8.29637303	-1.98214321	-0.04675783
H	10.26427744	-2.65153281	1.27934243
H	10.89570568	-5.05363890	1.47649049
H	9.50803789	-6.78121163	0.33631590
H	7.50306025	-6.11298137	-0.95294761
S	7.06196479	-0.69910145	-2.86125223
C	5.94391754	-1.24734940	-4.16204677
C	6.42280148	-2.17911231	-5.09226833
C	5.62537870	-2.55519139	-6.17481229
C	4.34240771	-2.02318474	-6.31729495
C	3.86710092	-1.10276760	-5.37967731
C	4.66272624	-0.69666533	-4.30661527
H	7.40921111	-2.61360499	-4.95786944
H	6.00252054	-3.27839255	-6.89472392
H	3.71694884	-2.32501810	-7.15457173
H	2.87335184	-0.67385355	-5.47772008
H	4.27231005	0.04597272	-3.61232412
S	6.14806926	1.93766594	-1.10862963
C	7.90207097	1.58177572	-0.88412442
C	8.81191227	2.15767059	-1.78293277
C	10.18597102	2.08301401	-1.54980058
C	10.67602539	1.41643197	-0.42581581
C	9.77668821	0.83587824	0.47258229
C	8.40223961	0.92892220	0.25422933
H	8.43344291	2.65183079	-2.67309267
H	10.87567471	2.53361347	-2.25995462
H	11.74675739	1.34950778	-0.24993706
H	10.14560473	0.32534777	1.35963226
H	7.70970492	0.50333737	0.97514079
O	3.71800628	2.48247278	-0.48658903
P	2.23920831	2.17387905	-1.65771074
O	2.93704433	1.44438235	-2.78091326
O	0.56785583	2.05484023	-1.98451400
C	0.10418082	2.38903067	-3.27525538
H	-0.92846727	2.02529873	-3.36612144
H	0.11239821	3.47617981	-3.43817094
H	0.71785329	1.91413637	-4.05168746
O	2.11792450	3.83036863	-1.84740481
C	3.29294618	4.61557893	-2.00188111
H	2.97294733	5.57515188	-2.42707499
H	3.78887326	4.78222015	-1.04103819
H	4.00524348	4.14056279	-2.68645231

Compound **8f**^{threo}: G_{THF} = -4503.160539 au

C	0.00000000	0.00000000	0.00000000
N	1.27590124	0.00000000	0.00000000
C	1.96485864	1.25274367	0.00000000
C	3.43772102	1.18849356	0.41481655
H	-0.58657586	0.93113719	0.01716223
H	1.39741712	2.05172318	0.49355044
H	3.77010511	0.17227144	0.18044293
C	-0.78302913	-1.24738442	-0.02773821
C	-0.15570726	-2.50439785	-0.09139548
C	-0.91338108	-3.67070189	-0.10190626
C	-2.31129509	-3.60818220	-0.05095385
C	-2.94419905	-2.36580422	0.00935957
C	-2.18424609	-1.19554716	0.02096024
H	0.92854564	-2.53123844	-0.13427893
H	-0.41571349	-4.63655852	-0.15245362
H	-2.90041380	-4.52231271	-0.06097162
H	-4.02968251	-2.30728353	0.04624987
H	-2.67693350	-0.22616137	0.06430147
C	3.84169810	1.44118452	1.87364639
C	3.38199634	2.55618155	2.61901787
C	3.50132423	2.57017059	4.02818202
C	4.32987601	1.62488180	4.67692067
C	4.98466074	0.63780051	3.90686343
C	4.70289248	0.51938125	2.52501236
S	2.64129410	3.98371275	1.78004188
C	4.11689017	4.91211348	1.30571502
C	4.37475558	5.12484025	-0.05353863
C	5.45706210	5.93304354	-0.41505098
C	6.28345416	6.50268066	0.55500383
C	6.02134613	6.27774031	1.90881601
C	4.93113065	5.49336251	2.28719252
H	3.75309382	4.64456906	-0.81004297
H	5.66067185	6.09963437	-1.47031765
H	7.12929493	7.12033532	0.25970502
H	6.65601561	6.72229057	2.67262756
H	4.70780207	5.33896610	3.33839143
S	2.67010813	3.81081723	5.03234523
C	0.94777514	3.62703098	4.58022651
C	0.14892018	4.77790636	4.60109658
C	-1.22097109	4.68336202	4.35739115
C	-1.80302624	3.44781631	4.06897954
C	-1.00466947	2.30252525	4.03856220
C	0.36161114	2.38442427	4.30686147
H	0.60583871	5.74517713	4.78967905
H	-1.82977005	5.58413615	4.37079812
H	-2.86771938	3.37844044	3.86220710
H	-1.44518190	1.33500250	3.81164337
H	0.97168957	1.48713184	4.29443747
S	4.52159394	1.63110413	6.46179222
C	5.47896893	3.10813943	6.78302651
C	6.34774448	3.68412715	5.84658382
C	7.10350700	4.80440451	6.19498275
C	7.01915198	5.34987068	7.47709579
C	6.15977612	4.76942832	8.41249991
C	5.38671477	3.66155294	8.06881612
H	6.43103259	3.26428940	4.84956099
H	7.76800389	5.24488824	5.45587891
H	7.61272750	6.22048288	7.74322679
H	6.07689515	5.18904880	9.41232851
H	4.70189321	3.22837318	8.79309954
S	6.24340516	-0.39867223	4.67154255
C	5.31418332	-1.68354470	5.49248244
C	5.96923124	-2.38667454	6.51568612
C	5.33060940	-3.44331518	7.16142853
C	4.02796109	-3.80494297	6.80918870
C	3.37429726	-3.10091886	5.79718230
C	4.01074062	-2.05059708	5.13393713
H	6.97519512	-2.09725552	6.80857926
H	5.85070347	-3.97783056	7.95298919
H	3.52822266	-4.62402897	7.31958297
H	2.36138541	-3.37206256	5.50992316
H	3.49552913	-1.52058028	4.33980575
S	5.46109942	-0.85167732	1.60485495
C	6.98257172	-0.10671502	0.98446470
C	8.19894758	-0.68502161	1.37026168
C	9.39965948	-0.19646188	0.85109631
C	9.38971361	0.88118881	-0.03558853
C	8.17442142	1.45928550	-0.41105940
C	6.96433823	0.96555173	0.08045038
H	8.19855716	-1.50612658	2.08052777
H	10.34102914	-0.65072762	1.15224388
H	10.32493480	1.26870517	-0.43344554
H	8.15812001	2.29631023	-1.10432746
H	6.02410771	1.41357330	-0.24220763
O	3.96896006	2.12696428	-0.49000592
P	2.53889653	2.05201046	-1.66736492
O	2.58154426	3.51057939	-2.07356520
O	1.00335825	1.58687051	-2.36431662
C	0.35456608	2.40006492	-3.31225987
H	-0.72050661	2.16628292	-3.28196524
H	0.50661620	3.46379826	-3.10238179
H	0.70738374	2.20625805	-4.34100247
O	3.43789810	0.95071288	-2.53231390
C	3.00996286	0.46741991	-3.79536187
H	3.80091568	-0.20213393	-4.15299508
H	2.06647385	-0.08190856	-3.72409836
H	2.89112475	1.28248236	-4.52215843

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