Electronic Supporting Information

"Reaction of Li/Cl phosphinidenoid complexes with phosphite substituted ketones: access to complexes with a novel mixed-valence polycyclic P,C-ligand system"

Liliya Abdrakhmanova, Arturo Espinosa and Rainer Streubel**

Content:

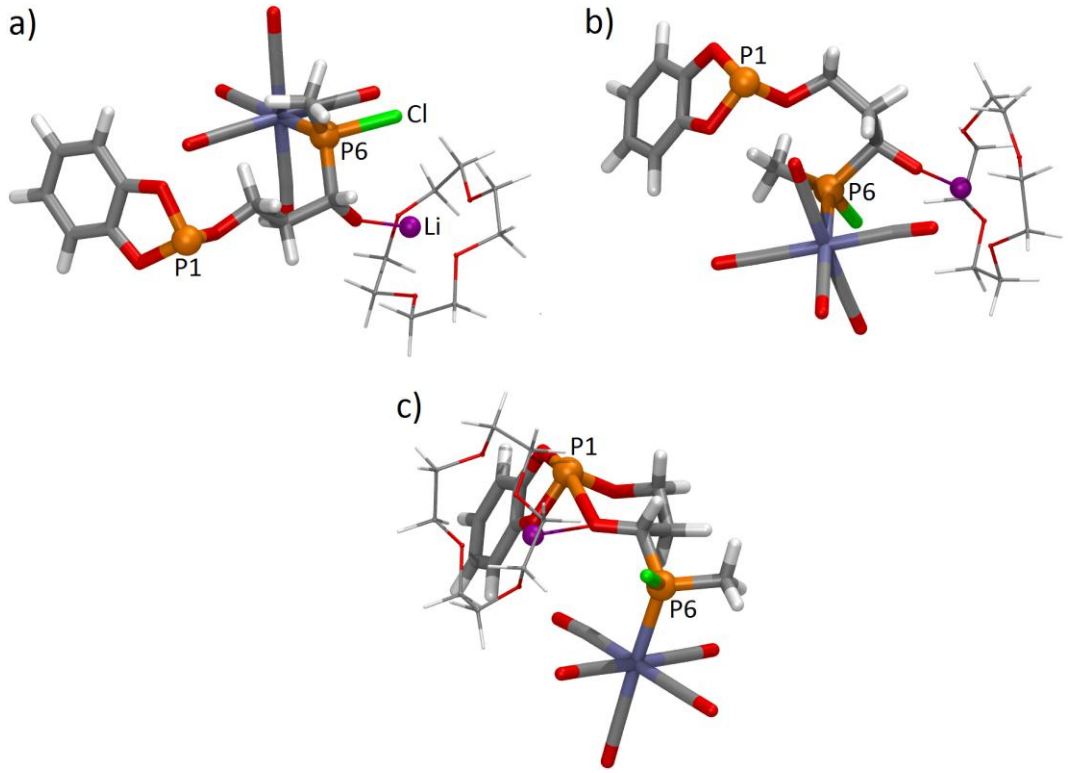

Figure S1: Calculated ($COSMO_{THF}$/B3LYP-D3/def2-SVP(ecp)) model structures for a) **5c**, b) **5c**^{conf} and c) **6c**.

Cartesian coordinates (Å) and energies (au) for all computed species.

Compound **2c**: E_{THF} = -2098.176422726 au

P	-0.205746	-0.072560	-0.109557	H	-1.259785	-4.998356	1.652924
W	2.411473	-0.176075	0.149503	H	0.190317	-4.889030	0.593359
C	4.434362	-0.251140	0.188154	O	-0.470410	-3.087955	1.427387
C	2.425407	0.387168	-1.858105	C	-0.269811	-2.950780	2.835753
C	2.354049	1.816179	0.698351	H	-0.856741	-3.716290	3.374133
C	2.397070	-0.699281	2.140683	H	0.794271	-3.070837	3.099629
C	2.175479	-2.181612	-0.332746	C	-0.758148	-1.566408	3.254767
O	5.595027	-0.279117	0.182557	H	-0.176449	-0.777195	2.748427
O	2.408107	0.731774	-2.955827	H	-0.643172	-1.434369	4.345596
O	2.265608	2.922835	1.016772	O	-2.125823	-1.498162	2.856447
O	2.437447	-0.999333	3.259228	C	-2.793682	-0.238650	2.823101
O	1.988221	-3.292985	-0.576249	H	-2.146877	0.526551	2.353352
C	-0.669998	1.647380	-0.651986	H	-3.065839	0.108870	3.836308
H	-0.019952	2.020878	-1.457725	C	-4.055404	-0.456531	1.995948
H	-1.720766	1.683043	-0.979101	H	-4.708928	-1.181120	2.513175
H	-0.545094	2.303622	0.226259	H	-4.606133	0.494900	1.888613
Cl	-0.621198	-1.061502	-2.048954	O	-3.670901	-0.975105	0.721026
Li	-1.868618	-1.791163	0.896160	C	-4.542544	-1.902490	0.071762
O	-2.749969	-3.424153	0.159253	H	-5.102651	-2.483516	0.826979
C	-1.647782	-4.193334	-0.316089	H	-5.266924	-1.377274	-0.575973
H	-1.117117	-3.648451	-1.116853	C	-3.677188	-2.845446	-0.757987
H	-1.977909	-5.172619	-0.706978	H	-3.137495	-2.286832	-1.545018
C	-0.742302	-4.383456	0.894999	H	-4.307766	-3.616738	-1.235865

Compound **3**^{mod}: E_{THF} = -990.574494578 au

C	0.222873	-0.079802	0.373332	C	-5.547929	-3.376746	-1.483972
O	1.431806	-0.097886	0.382715	C	-4.808250	-4.512127	-1.125184
H	-0.331472	0.862807	0.627279	O	-4.095038	-4.324720	0.037602
C	-0.629094	-1.279710	0.028473	C	-6.356579	-3.367005	-2.613526
H	-0.316039	-2.122361	0.667997	C	-6.416009	-4.543088	-3.381786
H	-0.392203	-1.577549	-1.008562	C	-5.679475	-5.678325	-3.020932
C	-2.119295	-1.021858	0.169730	C	-4.855386	-5.676344	-1.880532
H	-2.375128	-0.764101	1.214540	H	-6.925142	-2.474304	-2.881265
H	-2.430009	-0.173884	-0.463473	H	-7.046282	-4.566113	-4.274243
O	-2.826904	-2.194338	-0.253005	H	-5.745830	-6.582117	-3.631929
P	-4.171222	-2.713188	0.547507	H	-4.274022	-6.551602	-1.584178
O	-5.390724	-2.349944	-0.583987				

Compound **4c**·Li(12-c-4)Cl: E_{THF} = -3088.79090585 au

W	-0.705756	0.062510	-0.242952	H	-3.823920	-4.807665	1.938241
P	-0.276672	-0.054661	2.304620	C	-3.785578	-4.132339	3.989247
C	-0.840461	0.083957	-2.261181	H	-4.769191	-4.599818	4.174521
C	-2.718192	0.468190	-0.093136	H	-3.000394	-4.836248	4.319083
C	-0.472421	2.122000	-0.159175	O	-3.695541	-2.896926	4.698346
C	1.373259	-0.150053	-0.412037	C	-4.470006	-2.747441	5.885317
C	-1.075663	-1.978066	-0.149317	H	-5.289143	-3.488152	5.893920
O	-0.883024	0.079487	-3.419115	H	-3.848287	-2.908365	6.783947
O	-3.833302	0.766882	-0.041552	C	-5.079379	-1.342827	5.897582
O	-0.401383	3.269885	-0.101093	H	-4.317511	-0.563140	6.085327
O	2.514712	-0.181398	-0.522328	H	-5.843874	-1.267729	6.692211
O	-1.358548	-3.090713	-0.047214	C	-1.215935	-1.241777	3.475201
C	1.092884	0.964065	3.001994	O	-2.507642	-0.654880	3.390404
H	2.009463	0.723723	2.450743	H	-1.195398	-2.238861	3.026612
H	0.820948	2.022819	2.869695	C	-0.716035	-1.207418	4.922654
H	1.240573	0.756203	4.070781	H	0.383464	-1.172557	4.936337
Cl	1.448225	-2.014408	2.276304	H	-1.016783	-2.137844	5.429657
Li	-4.266087	-1.351583	3.287913	H	-2.341932	-0.355546	6.077747
O	-5.644018	-1.182709	4.608392	H	-0.745057	0.277116	6.534490
C	-6.443255	-0.061604	4.264905	C	-1.365911	-0.037876	5.684499
H	-5.850447	0.866523	4.334086	O	-1.568092	1.159138	4.891461
H	-7.319197	0.027169	4.931935	P	-2.007284	1.052023	3.313724
C	-6.914889	-0.333458	2.838294	O	-1.682979	2.735053	2.973906
H	-7.567078	-1.226040	2.849153	C	-2.813141	3.446096	2.732071
H	-7.506388	0.520811	2.460206	C	-3.963497	2.650067	2.820336
O	-5.778609	-0.579525	2.017593	O	-3.659046	1.356257	3.145230
C	-5.942564	-1.449841	0.899430	C	-2.910015	4.789738	2.386133
H	-6.859719	-2.051959	1.024090	C	-4.193300	5.313062	2.144184
H	-6.020973	-0.871754	-0.036386	C	-5.336453	4.509878	2.232866
C	-4.742679	-2.391576	0.839153	C	-5.232565	3.149130	2.569368
H	-3.824895	-1.867303	0.523727	H	-2.011210	5.402124	2.295563
H	-4.935105	-3.209456	0.122399	H	-4.296281	6.363850	1.862032
O	-4.601115	-2.876966	2.164053	H	-6.319981	4.937998	2.023437
C	-3.638313	-3.869218	2.491993	H	-6.108500	2.502625	2.619917
H	-2.622688	-3.519527	2.238025				

Compound **4c'**·Li(12-c-4)Cl: E_{THF} = -3088.784511792 au

W	-0.003246	0.102866	-0.132316	O	-0.984633	3.176615	0.061254
P	0.045753	0.048492	2.487817	O	3.056360	1.125759	-0.159701
C	-0.013406	0.241745	-2.141996	O	0.899613	-2.960256	-0.572006
C	-1.978077	-0.547156	-0.163009	C	0.706677	1.514383	3.393161
C	-0.638952	2.080279	0.018492	H	1.757442	1.668089	3.104459
C	1.970054	0.745259	-0.120575	H	0.102828	2.382239	3.101046
C	0.596714	-1.870661	-0.354380	H	0.637301	1.367650	4.481035
O	-0.009585	0.313023	-3.300298	Cl	-2.313592	1.012654	2.740144
O	-3.060161	-0.932754	-0.227144	Li	0.845200	-2.301139	6.238191

O	1.609595	-3.966988	6.919271	H	1.127389	-4.991516	5.176686
C	3.013159	-3.822119	6.718966	H	1.256423	-6.011883	6.637798
H	3.240342	-3.743909	5.640135	C	-0.553891	-1.227987	3.790506
H	3.569866	-4.680062	7.136090	O	0.642609	-1.560026	4.485849
C	3.395665	-2.545722	7.459150	H	-1.269987	-0.719279	4.444399
H	3.264007	-2.706439	8.544056	C	-1.131053	-2.463183	3.080243
H	4.455534	-2.294476	7.272872	H	-1.651696	-2.158129	2.160423
O	2.534800	-1.500338	7.020049	H	-1.868266	-2.962372	3.727909
C	2.156434	-0.509258	7.972173	H	0.179259	-4.082676	3.679531
H	2.276930	-0.903290	8.996378	H	-0.275366	-4.137499	1.961084
H	2.783447	0.393862	7.868709	C	-0.006715	-3.467094	2.789664
C	0.696413	-0.151943	7.736150	O	1.239167	-2.852513	2.397508
H	0.570038	0.302410	6.733809	P	1.767619	-1.444163	3.047253
H	0.355260	0.578836	8.489771	O	2.945673	-1.213368	1.771823
O	-0.036889	-1.373354	7.816983	C	4.212051	-1.419626	2.184870
C	-1.395156	-1.378282	7.385646	C	4.273840	-1.729928	3.551963
H	-1.496366	-0.825985	6.433479	O	3.027822	-1.761406	4.130023
H	-2.056486	-0.891644	8.124120	C	5.372133	-1.318525	1.422470
C	-1.805649	-2.834799	7.213644	C	6.602924	-1.536618	2.066223
H	-1.756520	-3.341936	8.192452	C	6.659821	-1.845177	3.430816
H	-2.845206	-2.883855	6.843811	C	5.483091	-1.943539	4.197079
O	-0.917684	-3.473597	6.296618	H	5.310744	-1.054869	0.364938
C	-0.556046	-4.829139	6.570964	H	7.527856	-1.455181	1.489208
H	-0.736443	-5.051472	7.636017	H	7.625838	-2.013224	3.913358
H	-1.159495	-5.527066	5.965617	H	5.513843	-2.184468	5.260274
C	0.926638	-5.025386	6.264172				

Compound **5c**: E_{THF} = -3088.777127063 au

W	0.445703	-0.137085	0.219494	H	5.194703	4.228468	1.980593
P	0.351062	-0.140919	2.762074	C	3.181942	4.471883	1.232272
C	0.503083	-0.205226	-1.811945	H	3.251162	5.574649	1.228375
C	-0.586640	1.662160	0.130293	H	3.433332	4.100804	0.223426
C	2.228701	0.945772	0.233825	O	1.865997	4.071800	1.606840
C	1.521356	-1.909454	0.366698	C	0.817024	5.019269	1.458173
C	-1.333633	-1.194616	0.257214	H	1.226078	6.043499	1.528038
O	0.517407	-0.237642	-2.968387	H	0.310662	4.911235	0.481820
O	-1.148511	2.665547	0.076409	C	-0.186727	4.795243	2.584418
O	3.221505	1.519602	0.150300	H	-0.741312	3.852361	2.441085
O	2.123783	-2.886199	0.469850	H	-0.914252	5.628448	2.609246
O	-2.324540	-1.780975	0.308101	C	1.979842	0.321301	3.714241
C	-0.439020	-1.622372	3.529198	O	2.315642	1.555356	3.377039
H	-1.523078	-1.592290	3.346015	H	1.659969	0.172273	4.782988
H	-0.031193	-2.521336	3.043961	C	3.090455	-0.694312	3.368166
H	-0.248695	-1.655196	4.613135	H	3.990365	-0.314080	3.879801
Cl	-0.926399	1.344342	3.587322	H	3.300316	-0.639320	2.287942
Li	1.943309	3.302777	3.549671	C	2.893597	-2.143312	3.775497
O	0.585997	4.740196	3.774251	H	2.662302	-2.224037	4.855085
C	-0.050728	4.563633	5.026882	H	2.071870	-2.624441	3.224416
H	-0.569229	3.589771	5.065305	O	4.099923	-2.854618	3.452386
H	-0.792892	5.360250	5.221268	P	4.529860	-4.225966	4.259950
C	1.066502	4.634396	6.062093	O	3.381579	-5.333337	3.656807
H	1.433003	5.674091	6.134101	C	3.779979	-5.781977	2.418069
H	0.678705	4.334016	7.053454	C	5.100787	-5.419541	2.117620
O	2.122619	3.779649	5.639956	O	5.696680	-4.705126	3.135594
C	3.459534	4.225136	5.855589	C	3.020527	-6.539175	1.537280
H	3.482811	5.327807	5.930260	C	3.623432	-6.930946	0.329329
H	3.869082	3.807482	6.793745	C	4.939536	-6.561539	0.026344
C	4.319924	3.785805	4.680010	C	5.700867	-5.791290	0.922711
H	4.282640	2.685231	4.575883	H	1.997121	-6.820006	1.792427
H	5.366444	4.102922	4.851734	H	3.050506	-7.528107	-0.384462
O	3.776732	4.400353	3.518305	H	5.386751	-6.875279	-0.919999
C	4.169391	3.903737	2.241272	H	6.725040	-5.486554	0.699313
H	4.117732	2.800599	2.233699				

Compound **5c'**: E_{THF} = -3088.766141317 au

W	-0.233036	1.307784	0.087141	H	0.567595	1.165266	9.463207
P	-0.540704	0.527346	2.579897	C	-1.485157	1.079915	8.778601
C	0.026766	1.860070	-1.843025	H	-1.824878	0.408439	9.587402
C	-1.859126	0.123834	-0.452099	H	-1.695114	2.122222	9.081617
C	-1.474673	2.959335	0.279578	O	-2.156411	0.752496	7.564784
C	1.479742	2.333203	0.611413	C	-3.461344	0.183013	7.654644
C	1.037816	-0.288275	-0.267924	H	-3.591317	-0.308563	8.635577
O	0.173018	2.179798	-2.945855	H	-4.242341	0.957285	7.545728
O	-2.731302	-0.553647	-0.770512	C	-3.595282	-0.859929	6.552070
O	-2.160619	3.884225	0.300917	H	-3.613282	-0.388615	5.551276
O	2.488082	2.828218	0.873288	H	-4.532405	-1.431615	6.683654
O	1.774164	-1.137566	-0.518848	C	-0.395209	1.505315	4.375650
C	0.484187	-0.947280	2.922550	O	0.027111	0.682647	5.310884
H	0.225379	-1.745803	2.213286	H	-1.467603	1.819814	4.462456
H	1.531479	-0.646973	2.754178	C	0.463946	2.775294	4.119532
H	0.355120	-1.270991	3.965068	H	1.340921	2.551620	3.486911
Cl	-2.492210	-0.310359	2.883887	H	0.854258	3.094387	5.099717
Li	-0.896826	-0.434717	6.447720	C	-0.374910	3.899842	3.513363
O	-2.451728	-1.692574	6.690090	H	-0.799914	3.590786	2.547173
C	-2.271101	-2.782120	5.802761	H	-1.222768	4.127102	4.176929
H	-2.313872	-2.434700	4.753654	O	0.310609	5.155336	3.346465
H	-3.045853	-3.557648	5.952649	P	1.512721	5.487585	2.268921
C	-0.899098	-3.344843	6.153883	O	0.710681	5.231703	0.775134
H	-0.941701	-3.786737	7.165505	C	0.087644	6.380255	0.351151
H	-0.612655	-4.135689	5.437672	C	0.407827	7.486253	1.151290
O	0.028761	-2.266175	6.137017	O	1.265558	7.162083	2.180462
C	1.133170	-2.305760	7.041275	C	-0.737715	6.506968	-0.759742
H	0.902239	-2.984514	7.880906	C	-1.233455	7.787127	-1.062599
H	2.038122	-2.680440	6.530423	C	-0.905713	8.893200	-0.269188
C	1.387946	-0.902014	7.584174	C	-0.073890	8.755605	0.857271
H	1.614596	-0.209929	6.753788	H	-0.984636	5.637813	-1.369925
H	2.240667	-0.921751	8.287636	H	-1.879688	7.918512	-1.934423
O	0.183881	-0.496828	8.237156	H	-1.299350	9.878817	-0.531011
C	0.006172	0.882856	8.553864	H	0.200406	9.606749	1.483473
H	0.345639	1.510230	7.709584				

Compound **5c^{conf}**: E_{THF} = -3088.778400923 au

W	-0.487422	0.514989	1.656727	C	-3.697245	-5.760675	3.865760
P	-1.083366	-0.726758	3.819835	H	-3.704106	-6.864768	3.875865
C	-0.064403	1.481161	-0.074706	H	-4.471033	-5.409707	4.573489
C	1.291895	-0.567482	1.535089	C	-4.043036	-5.250262	2.466933
C	-1.406536	-1.008521	0.538201	H	-4.201384	-4.159789	2.491716
C	-2.271785	1.551096	1.725659	H	-4.969160	-5.746710	2.120490
C	0.380913	2.025812	2.763672	O	-2.948643	-5.546147	1.604093
O	0.161772	2.039453	-1.064546	C	-2.936243	-4.899983	0.335005
O	2.255444	-1.189139	1.444651	H	-3.156848	-3.826252	0.462369
O	-1.870963	-1.754567	-0.202197	H	-3.678884	-5.349089	-0.351108
O	-3.264132	2.140560	1.711394	C	-1.538069	-5.083780	-0.242500
O	0.833590	2.889427	3.381828	H	-1.349534	-6.158225	-0.419372
C	-1.005792	0.116367	5.456612	H	-1.468030	-4.554577	-1.209289
H	0.045184	0.318938	5.706098	O	-0.584142	-4.574366	0.684552
H	-1.556646	1.057309	5.393168	C	0.654703	-5.263340	0.815149
H	-1.453160	-0.524075	6.232404	H	0.549563	-6.302349	0.455786
Cl	0.350393	-2.246547	4.298600	H	1.447532	-4.771574	0.223433
Li	-1.535022	-4.388608	2.527368	C	1.040269	-5.279636	2.289717
O	-0.107847	-5.765663	2.972062	H	1.301296	-4.265566	2.644916
C	-0.091410	-5.863771	4.388604	H	1.915235	-5.938037	2.443451
H	0.201143	-4.900830	4.843111	C	-2.612186	-1.914606	3.606418
H	0.619529	-6.638947	4.730407	O	-2.264695	-2.748044	2.629847
C	-1.506084	-6.249751	4.796612	H	-2.717032	-2.373521	4.626419
H	-1.735758	-7.248942	4.384411	C	-3.915637	-1.151326	3.265362
H	-1.579440	-6.301595	5.899193	H	-4.639484	-1.950886	3.029484
O	-2.412745	-5.287219	4.268264	H	-3.771588	-0.589903	2.328977

C	-4.554180	-0.261145	4.312380	C	-3.157164	2.910603	8.321995
H	-5.562039	0.044225	3.977142	C	-1.884340	3.351640	8.725285
H	-4.670773	-0.793327	5.272507	C	-0.933180	3.769397	7.785936
O	-3.744248	0.906572	4.548706	C	-1.222312	3.761899	6.410169
P	-4.417692	2.407394	4.677388	H	-3.907680	2.573271	9.039525
O	-4.617717	2.535499	6.368085	H	-1.633093	3.362645	9.789422
C	-3.437451	2.913016	6.961681	H	0.049829	4.104828	8.125231
C	-2.484595	3.334265	6.023583	H	-0.487276	4.057278	5.660190
O	-2.946636	3.243982	4.729089				

Compound **5c'**^{conf}: E_{THF} = -3088.775334816 au

W	-0.699632	-0.070433	0.725632	H	7.007333	4.178918	-1.962098
P	1.733827	0.133927	-0.125231	C	5.974318	3.217743	-3.612557
C	-2.633059	-0.347082	1.272273	H	6.038717	4.128870	-4.233158
C	-0.072577	-1.477382	2.129864	H	6.804040	2.546430	-3.895547
C	-0.521678	1.448095	2.118515	O	4.712498	2.581252	-3.817494
C	-1.277319	1.348762	-0.675602	C	3.973729	2.930728	-4.988899
C	-0.861286	-1.576350	-0.704583	H	4.217060	3.965154	-5.290546
O	-3.738399	-0.523779	1.568072	H	4.219727	2.258259	-5.830004
O	0.247698	-2.269884	2.898134	C	2.483735	2.843117	-4.675347
O	-0.460757	2.303346	2.891314	H	2.178088	1.801014	-4.471655
O	-1.601493	2.140439	-1.449238	H	1.902044	3.216257	-5.539008
O	-0.938500	-2.405235	-1.498488	C	3.006506	1.615852	0.164887
C	2.772562	-1.366839	-0.081313	O	3.833982	1.724110	-0.867022
H	2.294502	-2.186013	-0.634385	H	2.272371	2.450846	0.286774
H	3.751644	-1.126792	-0.520455	C	3.769181	1.470875	1.501968
H	2.892910	-1.657399	0.968984	H	4.421016	2.361192	1.521972
Cl	1.558456	0.300455	-2.252641	H	4.450639	0.606525	1.457709
Li	3.535823	2.965671	-2.155451	C	2.976125	1.439586	2.801823
O	2.286556	3.652846	-3.529735	H	3.568478	1.899528	3.613878
C	1.004748	3.808470	-2.942051	H	2.042607	2.014281	2.724650
H	0.626696	2.842130	-2.570765	O	2.617906	0.089814	3.169032
H	0.272240	4.217275	-3.663066	P	3.509320	-0.603158	4.382666
C	1.214822	4.799038	-1.802617	O	2.850076	-2.141618	4.239734
H	1.416355	5.798279	-2.228784	C	3.479720	-2.828869	3.224419
H	0.303548	4.861495	-1.180041	C	4.665982	-2.202793	2.813415
O	2.331915	4.368989	-1.030200	O	4.918232	-1.051384	3.522827
C	3.234802	5.368940	-0.565833	C	3.017896	-3.985282	2.614230
H	3.212001	6.237613	-1.248382	C	3.783672	-4.511116	1.559418
H	2.955584	5.720817	0.444639	C	4.967693	-3.887265	1.146272
C	4.645301	4.796453	-0.551894	C	5.427618	-2.715389	1.771370
H	4.715307	3.927844	0.124009	H	2.080155	-4.438315	2.937306
H	5.354268	5.573174	-0.208671	H	3.435577	-5.409882	1.044965
O	4.924384	4.396403	-1.886231	H	5.539026	-4.306357	0.314562
C	6.077355	3.607011	-2.141800	H	6.332793	-2.203027	1.440194
H	6.067609	2.711459	-1.493736				

Compound **6c**: E_{THF} = -3088.778940854 au

W	0.127204	-0.076953	-0.046887	H	1.628466	0.916604	4.273582
P	0.188186	-0.021799	2.500550	Cl	0.522902	-1.927591	3.385034
C	0.136199	-0.053680	-2.080993	Li	-3.770240	-0.979170	2.533655
C	-0.355934	-2.102891	-0.026070	O	-4.002194	-2.446104	4.043985
C	-1.890531	0.410892	-0.079001	C	-4.293751	-1.707843	5.221805
C	0.634673	1.931739	0.007479	H	-3.697196	-0.776921	5.228602
C	2.138753	-0.588430	-0.012715	H	-4.044468	-2.293675	6.128292
O	0.145608	-0.037041	-3.237309	C	-5.788420	-1.408176	5.219209
O	-0.593712	-3.227643	-0.026162	H	-6.345373	-2.354515	5.334166
O	-3.004289	0.677530	-0.184129	H	-6.029706	-0.768692	6.087335
O	0.926233	3.045221	0.067799	O	-6.180410	-0.755080	4.020443
O	3.253289	-0.876838	0.019248	C	-7.145175	-1.406390	3.209188
C	1.688119	0.816249	3.179251	H	-7.200983	-2.476695	3.473290
H	2.570260	0.218940	2.908929	H	-8.147999	-0.961887	3.361070
H	1.779992	1.808974	2.714570	C	-6.777089	-1.297549	1.739606

H	-6.829429	-0.256730	1.383171	H	-1.217504	2.439966	2.117530
H	-7.499833	-1.892069	1.149182	H	-0.191256	2.618190	3.564311
O	-5.469380	-1.817115	1.605288	C	-2.234124	3.092124	3.878552
C	-4.945143	-2.078967	0.315111	H	-2.333887	2.810462	4.944193
H	-4.577299	-1.148464	-0.154855	H	-1.944641	4.154185	3.839097
H	-5.704882	-2.521743	-0.356074	O	-3.496537	3.011868	3.215992
C	-3.815250	-3.081919	0.520619	P	-4.570337	1.826732	3.621268
H	-4.254265	-4.058089	0.787404	O	-5.981944	2.811249	3.459912
H	-3.231019	-3.204348	-0.408265	C	-6.391863	2.878406	2.160159
O	-2.972216	-2.629354	1.578852	C	-5.721781	1.951979	1.343698
C	-2.570405	-3.589272	2.557139	O	-4.839474	1.180405	2.051615
H	-3.232620	-4.468810	2.497235	C	-7.363308	3.727218	1.640776
H	-1.533441	-3.914890	2.370023	C	-7.664329	3.622340	0.270527
C	-2.685183	-2.965021	3.939702	C	-6.993044	2.701174	-0.542481
H	-1.956950	-2.150174	4.063555	C	-6.002252	1.853178	-0.013695
H	-2.482884	-3.737512	4.706966	H	-7.873714	4.440890	2.290830
C	-1.311390	0.729895	3.490325	H	-8.428415	4.273415	-0.162582
O	-2.505377	0.212602	3.186054	H	-7.243459	2.632172	-1.604527
H	-0.984099	0.546814	4.548041	H	-5.464037	1.137923	-0.635629
C	-1.163608	2.247690	3.203014				

Compound **6c'**: E_{THF} = -3088.781856772 au

W	0.062576	-0.130308	-0.260703	H	8.389882	-0.738570	-2.379705
P	2.590730	0.111298	0.242516	C	7.403169	1.028021	-1.595270
C	-1.897756	-0.161574	-0.794700	H	8.371511	1.563633	-1.566195
C	0.586827	-1.584934	-1.644866	H	6.871924	1.355315	-2.510221
C	-0.387895	-1.578843	1.152450	O	6.656057	1.311895	-0.429347
C	-0.207343	1.330968	1.196477	C	6.415058	2.695677	-0.187366
C	0.330670	1.338994	-1.710703	H	7.324314	3.282082	-0.420989
O	-3.007035	-0.157281	-1.121071	H	5.595160	3.055569	-0.834134
O	0.935985	-2.378342	-2.403683	C	6.049479	2.885050	1.269634
O	-0.704712	-2.374057	1.924767	H	5.294073	2.130706	1.532840
O	-0.297119	2.135515	2.013334	H	5.603547	3.890012	1.404192
O	0.426891	2.149543	-2.520503	C	3.520835	-0.432350	1.867495
C	3.724623	-0.434875	-1.082513	O	4.854893	-0.354003	1.785131
H	3.352652	-0.084494	-2.055136	H	3.060420	0.286577	2.594606
H	4.723503	-0.027838	-0.878892	C	2.980574	-1.838280	2.212034
H	3.750958	-1.535980	-1.074715	H	3.340718	-2.576482	1.474181
Cl	2.980980	2.203090	0.216666	H	1.881535	-1.844330	2.183371
Li	6.530400	-0.489564	1.074344	C	3.394627	-2.306540	3.605434
O	7.202877	2.734666	2.078666	H	3.295602	-1.482351	4.336180
C	7.063078	1.951218	3.250942	H	2.737725	-3.123003	3.939643
H	6.125332	1.368923	3.218531	O	4.721513	-2.857318	3.649158
H	7.048481	2.586905	4.158520	P	6.062131	-1.910540	3.614932
C	8.230091	0.986914	3.319963	O	7.127475	-3.033236	4.362192
H	9.183716	1.538216	3.388300	C	7.829455	-3.781019	3.456683
H	8.138620	0.347098	4.213312	C	7.575396	-3.391122	2.133705
O	8.239744	0.138418	2.169232	O	6.685047	-2.355648	2.057912
C	9.198466	0.465026	1.169642	C	8.731711	-4.800520	3.742036
H	8.927407	1.419811	0.693747	C	9.377435	-5.427703	2.660459
H	10.204173	0.574519	1.617119	C	9.116474	-5.038938	1.340840
C	9.240818	-0.686597	0.178669	C	8.202849	-4.006231	1.058636
H	9.586543	-1.594377	0.698170	H	8.931125	-5.096684	4.774233
H	9.954269	-0.454286	-0.630617	H	10.090895	-6.231269	2.861548
O	7.948944	-1.000358	-0.350999	H	9.629802	-5.540599	0.516979
C	7.616735	-0.480824	-1.633646	H	7.994083	-3.665488	0.043195
H	6.685902	-0.992438	-1.922681				

Compound **6c^{top}**: E_{THF} = -3088.781545189 au

W	-0.045788	-0.850848	0.928259	C	-0.775775	0.756569	-0.182470
P	0.399699	0.711464	2.882561	C	1.855673	-0.392477	0.245874
C	-0.384995	-2.145142	-0.604496	C	0.770832	-2.410026	2.019825
C	-1.940843	-1.275447	1.662046	O	-0.595067	-2.912296	-1.443645

O	-2.977620	-1.538629	2.085078	O	-3.833717	1.335823	0.860315
O	-1.125337	1.612199	-0.866260	C	-4.849736	0.926497	1.782638
O	2.915828	-0.117357	-0.113230	H	-5.763317	1.523159	1.620130
O	1.252324	-3.272230	2.612964	H	-5.091437	-0.140993	1.640384
C	2.024869	0.504886	3.715469	C	-4.370633	1.161616	3.205302
H	2.092993	-0.500241	4.155482	H	-3.477537	0.558894	3.438345
H	2.804001	0.606748	2.943403	H	-5.174754	0.869792	3.906762
H	2.167216	1.267159	4.495591	C	0.203844	2.571293	2.598476
Cl	-0.908818	0.460442	4.535274	O	-0.996372	2.857156	2.060492
Li	-2.751933	2.832046	1.899005	H	0.334483	2.982258	3.627076
O	-4.085800	2.549053	3.305177	C	1.395902	3.073304	1.736395
C	-3.753469	3.115163	4.571089	H	1.615342	2.383292	0.901871
H	-2.664716	3.041783	4.730525	H	2.307129	3.153732	2.353047
H	-4.271047	2.580765	5.387753	C	1.042963	4.424414	1.118259
C	-4.209015	4.581083	4.550698	H	1.923024	4.880815	0.638907
H	-5.295298	4.644880	4.743175	H	0.266934	4.279097	0.347759
H	-3.695564	5.121906	5.361825	O	0.576619	5.355661	2.109964
O	-3.894347	5.225466	3.324563	P	-1.062205	5.442188	2.376502
C	-4.945100	5.322498	2.375649	O	-1.097507	4.909145	4.013945
H	-5.676151	4.509888	2.523298	C	-1.033407	5.940721	4.898062
H	-5.472296	6.291550	2.484645	C	-1.032201	7.196596	4.268379
C	-4.406899	5.221546	0.958933	O	-1.076083	7.095094	2.911217
H	-3.632420	5.988265	0.776662	C	-1.002565	5.825812	6.282209
H	-5.243266	5.401659	0.259256	C	-0.986755	7.010706	7.041658
O	-3.875398	3.920056	0.764715	C	-0.993340	8.262459	6.417019
C	-3.837383	3.337840	-0.528399	C	-1.011677	8.370098	5.013468
H	-2.812616	3.402391	-0.929909	H	-0.996820	4.840173	6.752751
H	-4.513033	3.861912	-1.226389	H	-0.969053	6.945346	8.133148
C	-4.286611	1.869915	-0.384867	H	-0.984292	9.171972	7.023062
H	-5.386114	1.807428	-0.432627	H	-1.016990	9.339589	4.510817
H	-3.873108	1.269349	-1.211207				

Compound **6c'^{top}**: E_{THF} = -3088.781949924 au

W	0.192223	-0.523619	0.040492	O	8.524255	-0.946448	0.155339
P	2.712717	-0.289629	0.499493	C	8.040234	-0.541339	-1.117080
C	-1.778548	-0.580300	-0.462710	H	7.088467	-1.060916	-1.342426
C	0.740664	-0.608810	-1.953926	H	8.767691	-0.762236	-1.920236
C	0.245564	-2.595868	0.137614	C	7.816156	0.962634	-1.012541
C	-0.266898	-0.506362	2.075803	H	8.782044	1.453236	-0.797376
C	0.162938	1.551763	0.004006	H	7.430161	1.355513	-1.970122
O	-2.893088	-0.589156	-0.771845	O	6.894989	1.216677	0.043468
O	1.083566	-0.673692	-3.052720	C	7.150406	2.299249	0.931183
O	0.257345	-3.746456	0.184878	H	8.237693	2.486589	0.994217
O	-0.526715	-0.514975	3.195500	H	6.657721	3.225203	0.583736
O	0.164966	2.703053	-0.002001	C	6.633363	1.915551	2.314294
C	3.547000	0.975008	-0.523884	H	5.532104	1.826578	2.324205
H	3.093556	1.960848	-0.349035	H	6.934759	2.685350	3.050239
H	4.623746	0.980968	-0.300283	C	3.942076	-1.756556	0.488453
H	3.387821	0.692370	-1.577955	O	5.210383	-1.373956	0.595061
Cl	3.123194	0.459743	2.450144	H	3.545039	-2.318910	1.368784
Li	6.711779	-0.641845	1.175574	C	3.672581	-2.629025	-0.761663
O	7.235641	0.666257	2.598807	H	3.853798	-2.049624	-1.684798
C	6.891656	-0.063404	3.769009	H	2.636846	-2.998474	-0.785027
H	5.828832	-0.371366	3.730090	C	4.634233	-3.811771	-0.755902
H	7.057568	0.531529	4.686114	H	4.391863	-4.523803	-1.560075
C	7.812650	-1.281708	3.769980	H	5.665303	-3.447731	-0.901955
H	8.849601	-0.954574	3.969285	O	4.541199	-4.539677	0.484414
H	7.504554	-1.985835	4.564179	P	5.719127	-4.414083	1.633048
O	7.734541	-1.894032	2.490650	O	4.888475	-3.632570	2.897516
C	8.907909	-2.442135	1.914208	C	4.129254	-4.523531	3.611035
H	9.795057	-1.868946	2.240122	C	4.445381	-5.855018	3.298494
H	9.046878	-3.499958	2.205587	O	5.426873	-5.941917	2.341867
C	8.755418	-2.323826	0.405346	C	3.156314	-4.213628	4.554126
H	7.898313	-2.930491	0.061264	C	2.505375	-5.282262	5.197535
H	9.666654	-2.688231	-0.104899	C	2.825884	-6.610544	4.890446

C	3.806469	-6.916171	3.927344	H	2.303775	-7.424111	5.400212
H	2.909874	-3.173691	4.778931	H	4.065150	-7.945278	3.668381
H	1.735693	-5.065781	5.943481				