Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Supporting Information

Experimental and computational study of the ring opening of tricyclic oxanorbornenes to polyhydro isoindole phosphonates

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D.D.C. and B.I.R. are Ph.D. fellows of the Research Foundation – Flanders (FWO - Vlaanderen).

Table of contents supporting information

Computational data

Cartesian coordinates of the reported structures

Structure of the files:

Number of atoms

Energy in au negative frequencies

xyz-coordinates in Å

Coordinates in Å calculated at B3LYP/BS_1

Complex C**1**

42
scf done: -4518.20413852 no negative frequencies

C	-0.359297	3.529443	0.227942
C	0.730206	2.552852	0.738601
C	-0.143184	1.452306	1.435857
O	-1.278326	1.433258	0.530219
C	-1.657363	2.820761	0.743036
C	1.498127	1.735997	-0.305793
N	1.720459	0.425875	0.373511
C	0.708848	0.185524	1.424367
C	-1.684158	2.892996	2.261742
C	-0.759203	2.031187	2.694365
P	-0.320468	-1.351268	1.27111
O	0.532293	-2.688336	1.269545
C	0.994097	-3.367362	0.072309
C	2.867808	-0.306281	0.470435
C	4.042199	-0.027706	-0.542543
Cl	4.895497	1.486385	-0.015955
O	3.013174	-1.18023	1.308601
O	-0.971443	-1.323746	2.716875
C	-1.924403	-2.330499	3.156915
O	-1.268041	-1.353452	0.085442
Cl	5.203014	-1.378875	-0.476324
Cl	3.451212	0.140615	-2.229202
H	1.21754	0.068968	2.388454
H	0.869221	-4.434015	0.261934
H	0.403527	-3.06776	-0.795632
H	2.049561	-3.128165	-0.061114
H	-2.152813	-2.079716	4.192315
H	-2.824955	-2.270633	2.544269
H	-1.465324	-3.320149	3.100649
H	2.449114	2.192176	-0.568818
H	0.908964	1.57419	-1.210045

H	1.423629	3.012058	1.449417
H	-0.246409	4.543596	0.618722
H	-0.379263	3.57486	-0.864522
H	-2.574146	3.041133	0.203595
H	-2.28858	3.580066	2.841281
H	-0.415679	1.840392	3.703608
Ti	-2.602816	-0.283104	-1.002944
Cl	-3.570917	-1.907884	-2.097016
Cl	-3.64728	1.532887	-1.793418
Cl	-0.823769	0.016371	-2.43282
Cl	-3.922577	-0.343974	0.870063

TS **1**

42

scf done: -4518.16282729 one negative frequency

C	0.461740	-3.107302	1.368613
C	-0.637929	-2.027197	1.479129
C	0.036605	-0.725036	1.842750
O	1.408449	-1.238399	0.404485
C	1.772494	-2.287542	1.305466
C	-1.434449	-1.632501	0.221883
N	-1.820913	-0.222385	0.515562
C	-0.825332	0.405180	1.395924
C	2.004695	-1.598685	2.642844
C	1.023697	-0.710940	2.899677
P	0.187619	1.775995	0.640631
O	-0.813013	2.813436	-0.018442
C	-1.043581	2.898019	-1.454862
C	-3.050225	0.384104	0.465648
C	-4.174810	-0.279073	-0.412106
Cl	-4.825671	-1.711064	0.496518
O	-3.289553	1.418814	1.057724
O	0.686938	2.459521	1.988749
C	1.813566	3.389694	1.970265
O	1.252802	1.331105	-0.313354
Cl	-5.497592	0.884159	-0.657946
Cl	-3.543600	-0.791508	-2.014812
H	-1.321972	0.882089	2.257510
H	-0.931605	3.948946	-1.725646
H	-0.324173	2.284036	-1.999756
H	-2.065848	2.566909	-1.643761
H	1.920596	3.730035	3.000924
H	2.710061	2.864579	1.638387
H	1.582956	4.234577	1.319988
H	-2.316003	-2.252513	0.076386
H	-0.803649	-1.663135	-0.669958
H	-1.347245	-2.252136	2.292779
H	0.439979	-3.811064	2.206042
H	0.349169	-3.674228	0.439324

H	2.632415	-2.848326	0.939580
H	2.875969	-1.765679	3.266257
H	1.038109	0.049508	3.676719
Ti	2.620022	-0.226171	-0.866805
Cl	3.808677	1.299510	-1.987293
Cl	3.867845	-2.033350	-1.291864
Cl	1.089495	-0.607047	-2.565318
Cl	3.819401	0.309556	1.166992

Complex C**3**

42

scf done: -4518.230078 no negative frequencies

C	-0.430193	3.207561	-0.002042
C	0.646831	2.336403	0.699703
C	0.095143	1.404609	1.760569
O	-2.146249	1.549678	-0.156905
C	-1.858244	2.809749	0.398262
C	1.466772	1.401140	-0.208714
N	1.941438	0.363677	0.733711
C	0.932197	0.139321	1.781902
C	-1.947046	2.739090	1.941418
C	-1.048539	1.622500	2.412860
P	-0.158234	-1.293273	1.322004
O	0.733547	-2.585757	1.037872
C	1.054045	-3.066013	-0.291898
C	3.156040	-0.239527	0.891554
C	4.281497	0.052243	-0.171715
Cl	4.829571	1.771157	0.009388
O	3.400097	-0.989648	1.818228
O	-0.841906	-1.595639	2.729697
C	-1.822576	-2.657314	2.884753
O	-1.070761	-0.985041	0.163058
Cl	5.668035	-1.019880	0.123061
Cl	3.675366	-0.233112	-1.847622
H	1.425528	-0.097854	2.728328
H	0.947598	-4.151475	-0.262960
H	0.377248	-2.637926	-1.034035
H	2.089417	-2.800080	-0.513925
H	-2.133868	-2.618849	3.928394
H	-2.673431	-2.477471	2.224582
H	-1.355621	-3.621033	2.667366
H	2.298928	1.912553	-0.685182
H	0.843051	0.941970	-0.983335
H	1.363761	3.004333	1.198582
H	-0.283785	4.264037	0.248653
H	-0.347650	3.122575	-1.090789
H	-2.587184	3.528602	0.007498
H	-1.680162	3.719535	2.349438
H	-1.431109	0.933041	3.157548

Ti	-2.609038	0.078513	-0.981907
Cl	-4.015527	-1.327109	0.062898
Cl	-4.189748	0.995979	-2.273820
Cl	-1.242684	-0.432873	-2.700404
Cl	-3.654482	2.452345	2.482955

Complex C**2**

43

scf done: -4978.507403 no negative frequencies

C	-1.027032	1.988700	2.550898
C	-0.281232	1.464066	1.345363
C	0.547394	2.620232	0.708580
C	-0.566406	3.529521	0.133555
C	-1.849070	2.733169	0.543816
C	-1.986817	2.775266	2.053789
O	-1.362671	1.368081	0.336005
C	0.680796	0.286964	1.423236
N	1.676101	0.554113	0.359323
C	1.417374	1.864811	-0.300394
C	2.830042	-0.158271	0.410110
O	2.987067	-1.123069	1.139146
P	-0.244878	-1.297894	1.406942
O	-1.331137	-1.377155	0.328797
Ti	-2.491174	-0.336584	-0.882086
Cl	-4.036172	-0.205168	0.836786
O	0.592664	-2.647777	1.358442
C	1.039393	-3.267893	0.128291
O	-0.826476	-1.275393	2.883218
C	-1.897091	-2.162864	3.282481
C	4.022980	0.244542	-0.549272
Cl	3.469507	0.450791	-2.257207
Cl	4.801167	1.759471	0.045027
Cl	5.252495	-1.059689	-0.528483
Cl	-3.450711	-2.085315	-1.861601
Cl	-3.492734	1.343239	-2.037213
Cl	-0.662293	-0.300184	-2.325232
H	1.189144	0.382804	2.412114
H	0.917978	-4.343372	0.270004
H	0.437693	-2.933754	-0.720317
H	2.091006	-3.015813	-0.009278
H	-2.083926	-1.937631	4.332556
H	-2.787577	-1.960618	2.683588
H	-1.580134	-3.204161	3.175305
H	2.353260	2.382267	-0.496764
H	0.891285	1.687583	-1.241384
H	1.165528	3.075409	1.485916
H	-0.556084	4.536914	0.557969
H	-0.509135	3.606720	-0.957096
H	-2.735379	2.903883	-0.059835

H	-2.673963	3.418007	2.590921
H	-0.673319	1.843780	3.562968
Cl	2.079806	1.927192	3.848624

TS **2**

43

scf done: -4978.477537 one negative frequency

C	-0.834579	1.851753	2.625170
C	-0.016958	1.399656	1.531971
C	0.736059	2.457579	0.714238
C	-0.333719	3.410702	0.135409
C	-1.643862	2.772422	0.628829
C	-1.735005	2.762620	2.152627
O	-1.381712	1.359515	0.299774
C	0.834959	0.153859	1.541647
N	1.871142	0.384780	0.523458
C	1.564090	1.616988	-0.264988
C	3.058405	-0.246827	0.736683
O	3.253831	-1.004174	1.671983
P	-0.158278	-1.396503	1.342426
O	-1.404062	-1.311193	0.502699
Ti	-2.540013	0.017778	-0.645838
Cl	-4.023565	0.096667	1.140279
O	0.819497	-2.545347	0.831900
C	0.630805	-3.201570	-0.454614
O	-0.473980	-1.705264	2.879749
C	-1.713972	-2.365111	3.247835
C	4.234708	0.004507	-0.283484
Cl	3.676949	-0.031636	-1.990271
Cl	4.989982	1.611902	0.095720
Cl	5.478693	-1.261855	-0.066809
Cl	-3.599394	-1.785111	-1.560916
Cl	-3.565737	1.617274	-1.848639
Cl	-0.755970	-0.227685	-2.249161
H	1.309619	0.037578	2.524019
H	-0.079322	-4.022958	-0.334391
H	0.265317	-2.497428	-1.204325
H	1.614031	-3.586579	-0.727615
H	-1.761805	-2.306796	4.335603
H	-2.563013	-1.849098	2.794335
H	-1.688446	-3.412087	2.932330
H	2.483001	2.114235	-0.566708
H	0.984061	1.337087	-1.147097
H	1.397952	2.986067	1.411009
H	-0.233640	4.428947	0.511733
H	-0.321794	3.390571	-0.959109
H	-2.541343	3.114818	0.121290
H	-2.581773	3.149719	2.694290
H	-0.801427	1.428067	3.621107

Cl	-1.112461	5.307046	2.723458

Complex C**4**

43

scf done: -4978.551492 no negative frequencies

C	-0.803675	1.770373	2.511233
C	0.309582	1.498512	1.825922
C	0.859815	2.371118	0.717896
C	-0.189356	3.275193	0.022572
C	-1.625566	3.015708	0.507584
C	-1.709537	2.862133	2.044417
O	-2.118199	1.842467	-0.053163
C	1.099532	0.203240	1.862882
N	2.091090	0.360967	0.786888
C	1.603314	1.370452	-0.185799
C	3.284503	-0.266261	0.934087
O	3.570567	-0.957843	1.897018
P	-0.087942	-1.168326	1.446376
O	-1.137518	-0.761047	0.470901
Ti	-2.788870	0.280897	-0.626872
Cl	-3.985471	0.082252	1.467070
O	0.760956	-2.426118	0.922267
C	0.557924	-2.955344	-0.417261
O	-0.586506	-1.568448	2.916577
C	-1.778205	-2.390504	3.058690
C	4.365540	-0.080187	-0.202525
Cl	3.684899	-0.426953	-1.832136
Cl	5.004609	1.621403	-0.144156
Cl	5.730976	-1.193465	0.090296
Cl	-3.405326	-1.945909	-1.133310
Cl	-4.492801	1.194637	-1.795153
Cl	-1.211567	0.239751	-2.425114
H	1.602291	-0.032415	2.803707
H	0.711589	-4.033498	-0.338957
H	-0.447345	-2.729670	-0.779163
H	1.302683	-2.518802	-1.087032
H	-1.936446	-2.490848	4.133470
H	-2.630005	-1.897161	2.584316
H	-1.602432	-3.375652	2.616367
H	2.428669	1.830072	-0.723754
H	0.920345	0.901777	-0.903785
H	1.623495	3.015073	1.179790
H	0.054146	4.326526	0.203244
H	-0.179911	3.109299	-1.059444
H	-2.270244	3.849198	0.196384
H	-2.738459	2.648137	2.328449
H	-1.171576	1.106219	3.287349
Cl	-1.332299	4.497965	2.859482

Complex C**5**

41
scf done: -4123.251819 no negative frequencies

C	-0.287654	3.454615	0.539037
C	0.799079	2.410826	0.814065
C	-0.057311	1.175492	1.271983
C	-1.385519	1.267392	0.517590
N	-1.398736	2.641275	-0.025706
C	1.700378	2.625678	2.056777
C	1.195653	1.464919	2.985684
C	1.627536	0.138327	2.368271
C	0.834897	-0.051736	1.307628
O	-0.209495	1.480534	2.667472
P	-2.815875	0.896381	1.643481
O	-2.356060	-0.495464	2.240866
C	-3.159894	-1.246140	3.190233
C	-2.232602	2.882085	-1.072195
C	-2.211687	4.300399	-1.755792
Cl	-3.561339	4.416995	-2.912045
O	-3.000545	2.032637	-1.497930
O	-3.106762	2.038103	2.610008
Fe	-2.639508	2.826054	4.347697
O	-4.134166	0.524806	0.837197
C	-5.233880	1.438768	0.581410
Cl	-2.381124	5.610379	-0.536215
Cl	-0.656432	4.483586	-2.672457
H	-1.445827	0.547537	-0.305088
H	-6.127496	0.816235	0.527905
H	-5.324032	2.160713	1.395349
H	-5.054415	1.934458	-0.372603
H	-2.658215	-2.207189	3.298523
H	-3.176249	-0.720190	4.146368
H	-4.168782	-1.389472	2.796086
H	0.028293	4.215007	-0.170112
H	-0.624483	3.937565	1.460091
H	1.360716	2.196547	-0.099907
H	2.767472	2.559294	1.830301
H	1.500818	3.587487	2.536997
H	1.341512	1.606278	4.054912
H	2.476942	-0.454491	2.686291
H	0.879022	-0.824963	0.550000
Cl	-4.611964	3.530223	5.090035
Cl	-1.841558	1.267247	5.725350
Cl	-1.260228	4.562768	4.118928

TS **3**

41
scf done: -4123.20045224 one negative frequency

C	-0.542986	3.434610	0.630269

C	0.565776	2.411465	0.935641
C	-0.174860	1.110682	0.999959
C	-1.470613	1.233355	0.312223
N	-1.489815	2.621835	-0.169546
C	1.462982	2.603783	2.178495
C	1.012631	1.545739	3.197864
C	1.186922	0.151358	2.618916
C	0.479259	-0.064360	1.479355
O	-0.394317	1.666868	3.306217
P	-2.917838	0.890067	1.502053
O	-2.479068	-0.577880	1.953512
C	-3.197498	-1.249752	3.028123
C	-2.167705	2.876503	-1.323614
C	-2.118843	4.332440	-1.915148
Cl	-3.251946	4.453426	-3.280317
O	-2.802020	2.012551	-1.905973
O	-3.108521	1.966281	2.504114
Fe	-1.400188	2.631011	4.633388
O	-4.173196	0.598480	0.554146
C	-5.207627	1.583244	0.303525
Cl	-2.561795	5.549090	-0.672353
Cl	-0.436853	4.641174	-2.532403
H	-1.607212	0.522443	-0.512220
H	-6.155521	1.042980	0.319300
H	-5.200350	2.353270	1.077785
H	-5.035854	2.014150	-0.684231
H	-2.657016	-2.179768	3.204936
H	-3.193387	-0.626048	3.924711
H	-4.218918	-1.467220	2.705056
H	-0.173102	4.285108	0.065016
H	-1.030610	3.784771	1.545010
H	1.190961	2.314752	0.030467
H	2.527254	2.517292	1.935329
H	1.291331	3.596253	2.608509
H	1.507813	1.669164	4.164193
H	1.681839	-0.648266	3.162953
H	0.263347	-1.046755	1.072134
Cl	-2.935928	1.417591	5.736143
Cl	0.267642	2.968389	6.145314
Cl	-1.943691	4.700891	3.937637

Complex C**6**

41

scf done: -4123.232312 no negative frequencies

C	-0.999643	3.497556	0.350862
C	0.074132	2.716758	1.126638
C	-0.553796	1.344136	1.300126
C	-1.684368	1.190845	0.304906

N	-1.616989	2.443018	-0.477034
C	0.527446	3.325278	2.463037
C	1.288359	2.291166	3.283389
C	0.946603	0.864985	3.141692
C	-0.147606	0.472231	2.231083
O	0.497901	1.649271	4.343516
P	-3.342236	1.092772	1.155708
O	-3.127384	-0.259969	1.998060
C	-4.156851	-0.699998	2.912084
C	-1.976907	2.407158	-1.788142
C	-1.824642	3.722575	-2.643599
Cl	-2.504954	3.459284	-4.264252
O	-2.411570	1.402704	-2.325011
O	-3.690216	2.340227	1.886895
Fe	1.121247	1.332442	6.259347
O	-4.414281	0.613116	0.055951
C	-5.290917	1.536502	-0.623948
Cl	-2.700456	5.095522	-1.864817
Cl	-0.063285	4.122063	-2.817089
H	-1.581582	0.331792	-0.363591
H	-6.264286	1.047864	-0.700538
H	-5.385471	2.466964	-0.058713
H	-4.890553	1.725122	-1.622256
H	-3.726888	-1.524765	3.481142
H	-4.437357	0.112757	3.587122
H	-5.028937	-1.046719	2.350717
H	-0.583042	4.295645	-0.256348
H	-1.758351	3.907985	1.026144
H	0.947073	2.605810	0.465593
H	1.159580	4.203884	2.298444
H	-0.344991	3.649466	3.041316
H	2.291969	2.539610	3.619643
H	1.692568	0.125577	3.421862
H	-0.613228	-0.498187	2.363805
Cl	-0.143735	-0.312115	6.977547
Cl	3.242542	0.767443	5.903947
Cl	0.865578	3.283195	7.231248

TS **4**

41

scf done: -4123.213903 one negative frequency

C	1.574195	1.368066	4.693188
C	0.779311	1.361104	3.562365
C	0.833388	2.468141	2.551258
C	0.961788	3.842452	3.233099
C	2.076390	3.844297	4.305851
C	2.334561	2.504997	4.931307
C	-0.400150	2.215452	1.664026
N	-0.565844	0.754124	1.780557

C	-0.190876	0.330544	3.130726
O	1.632289	4.557716	5.423430
Fe	2.147458	4.675505	7.225937
Cl	4.392063	4.463035	7.186933
P	-1.755113	0.290282	4.252278
O	-2.871523	1.033769	3.619246
C	-1.137539	-0.174098	0.967302
C	-1.540559	0.250175	-0.489699
Cl	-2.750249	1.581107	-0.434777
O	-2.017480	-1.251594	4.603682
C	-3.046944	-2.022880	3.930076
O	-1.105069	0.845345	5.598710
C	-1.883439	1.017419	6.815607
O	-1.303520	-1.326812	1.331556
Cl	1.399331	6.560690	8.108801
Cl	1.290848	2.801220	8.206106
Cl	-0.056081	0.789791	-1.383079
Cl	-2.242163	-1.141261	-1.340570
H	0.200578	-0.691816	3.139308
H	-3.208375	-2.901149	4.555883
H	-3.964545	-1.436417	3.850533
H	-2.694884	-2.313178	2.939391
H	-1.228616	1.551521	7.503666
H	-2.778171	1.607220	6.602491
H	-2.152696	0.037140	7.215865
H	-0.243037	2.519809	0.632236
H	-1.289842	2.718209	2.060469
H	1.734295	2.276841	1.945129
H	1.138632	4.626098	2.490638
H	0.024701	4.074704	3.748740
H	3.014302	4.261241	3.905556
H	3.097728	2.499373	5.706483
H	1.604686	0.525648	5.375668

Complex C**7**

41

-4123.23247707 no negative frequencies

C	2.7091	1.4292	4.2784
C	1.6187	1.3346	3.5045
C	1.2182	2.3833	2.4901
C	1.7786	3.7608	2.8435
C	3.2914	3.6169	3.0736
C	3.5972	2.6142	4.2028
C	-0.3049	2.2034	2.4079
N	-0.4366	0.7365	2.5383
C	0.5619	0.2455	3.5139
O	3.9007	4.8518	3.2874
Fe	4.6245	5.5740	4.7768
Cl	6.7594	5.1457	5.1246

P	-0.2592	0.0718	5.1779
O	-0.9974	1.2922	5.5964
C	-1.1218	-0.1813	1.8041
C	-2.1202	0.3351	0.6982
Cl	-3.2883	1.5234	1.3903
Cl	3.4307	3.5834	5.8760
O	-1.1259	-1.2834	5.1410
C	-2.5524	-1.2840	4.9206
O	1.0097	-0.4019	6.0508
C	0.8327	-0.6934	7.4543
O	-1.0014	-1.3829	1.9715
Cl	3.8045	7.4608	5.5364
Cl	-1.1734	1.0984	-0.6480
Cl	-3.0328	-1.0395	0.0354
H	0.9270	-0.7374	3.2016
H	-2.9755	-2.0306	5.5957
H	-2.9774	-0.3013	5.1396
H	-2.7436	-1.5704	3.8843
H	1.8290	-0.8844	7.8546
H	0.3824	0.1613	7.9664
H	0.2058	-1.5812	7.5746
H	-0.7232	2.5664	1.4741
H	-0.8153	2.6827	3.2501
H	1.6273	2.0747	1.5136
H	1.6122	4.4824	2.0376
H	1.3065	4.1545	3.7514
H	3.7400	3.1633	2.1716
H	4.6600	2.3708	4.2415
H	2.9524	0.6641	5.0078

TS **5**

41

-4123.20951729 one negative frequency

C	-1.0616	3.5014	0.4143
C	-0.0587	2.7040	1.2639
C	-0.6831	1.3377	1.3597
C	-1.7343	1.1883	0.2990
N	-1.6296	2.4517	-0.4562
C	0.3318	3.2632	2.6359
C	1.1088	2.2211	3.4372
C	0.6896	0.8489	3.2727
C	-0.2566	0.4370	2.2788
O	1.7273	2.6559	4.5137
P	-3.4414	1.0509	1.0684
O	-3.2033	-0.2614	1.9614
C	-4.2490	-0.7229	2.8508
C	-1.9427	2.4340	-1.7813
C	-1.7516	3.7553	-2.6155
Cl	-2.3676	3.5107	-4.2632

O	-2.3597	1.4333	-2.3388
O	-3.8563	2.3115	1.7362
Fe	1.6920	1.8054	6.2355
O	-4.4287	0.4958	-0.0678
C	-5.2988	1.3600	-0.8343
Cl	-2.6506	5.1211	-1.8541
Cl	0.0173	4.1443	-2.7101
H	-1.5898	0.3338	-0.3689
H	-6.2377	0.8190	-0.9640
H	-5.4779	2.2967	-0.3010
H	-4.8353	1.5443	-1.8052
H	-3.8045	-1.5128	3.4562
H	-4.5862	0.0948	3.4925
H	-5.0828	-1.1207	2.2662
H	-0.5890	4.2908	-0.1626
H	-1.8577	3.9251	1.0358
H	0.8674	2.5776	0.6706
H	0.9309	4.1731	2.5439
H	-0.5572	3.5049	3.2345
H	1.9019	1.6472	2.6677
H	1.1627	0.1158	3.9226
H	-0.6220	-0.5829	2.3089
Cl	-0.4588	1.1043	6.2650
Cl	3.0008	-0.0043	6.0301
Cl	2.2607	3.2220	7.8197

Complex C**8**

41

-4123.27611649 no negative frequencies

C	-1.1754	3.5233	0.5451
C	-0.2010	2.7633	1.4616
C	-0.7450	1.3476	1.4678
C	-1.7103	1.1823	0.3097
N	-1.6023	2.4744	-0.4006
C	-0.0899	3.2981	2.8957
C	0.6577	2.3309	3.7741
C	0.4818	0.8476	3.5627
C	-0.4429	0.4770	2.4316
O	1.3899	2.7753	4.6720
P	-3.4511	0.9682	0.9290
O	-3.3029	-0.4653	1.6481
C	-4.4582	-1.0773	2.2599
C	-1.7946	2.4902	-1.7480
C	-1.5977	3.8515	-2.5197
Cl	-2.0468	3.6364	-4.2256
O	-2.1104	1.4972	-2.3797
O	-3.9151	2.1263	1.7415
Fe	2.5421	1.9031	6.1154
O	-4.3859	0.5853	-0.3242

C	-5.2042	1.5551	-1.0103
Cl	-2.6412	5.1430	-1.8067
Cl	0.1455	4.3418	-2.4404
H	-1.4675	0.3659	-0.3751
H	-6.1419	1.0548	-1.2604
H	-5.4026	2.4173	-0.3690
H	-4.6930	1.8588	-1.9264
H	-4.0964	-1.9701	2.7713
H	-4.9147	-0.3938	2.9814
H	-5.1842	-1.3560	1.4914
H	-0.7062	4.3590	0.0343
H	-2.0488	3.8788	1.1027
H	0.7923	2.7719	0.9889
H	0.3789	4.2836	2.9673
H	-1.1043	3.3725	3.3213
H	1.4923	0.4234	3.4333
H	0.1391	0.4262	4.5203
H	-0.8665	-0.5219	2.4449
Cl	1.0890	0.6876	7.2582
Cl	3.9675	0.6842	4.9411
Cl	3.4439	3.5584	7.2336

Coordinates in Å calculated at TPSSh/BS_3

Complex C**1**

42

scf done: -5309.697831 no negative frequencies

C	-0.340366	3.526947	0.221573
C	0.727210	2.535403	0.741749
C	-0.162432	1.426857	1.397930
O	-1.259952	1.417302	0.428008
C	-1.655342	2.808823	0.664456
C	1.495651	1.726111	-0.308443
N	1.722496	0.418822	0.373535
C	0.708211	0.175196	1.419968
C	-1.746593	2.845164	2.176708
C	-0.835537	1.978349	2.632897
P	-0.292771	-1.373305	1.287804
O	0.565992	-2.707982	1.266883
C	0.984840	-3.371012	0.037934
C	2.870733	-0.308463	0.484626
C	4.045408	-0.021298	-0.518254
Cl	4.876244	1.500443	0.010140
O	3.011372	-1.182731	1.328942
O	-0.911361	-1.346169	2.750315
C	-1.883861	-2.346941	3.179849
O	-1.258697	-1.368131	0.118289
Cl	5.212285	-1.358196	-0.438868
Cl	3.461357	0.141470	-2.203682
H	1.210725	0.095613	2.392079

H	0.872218	-4.438260	0.226515
H	0.355012	-3.060493	-0.797317
H	2.031845	-3.119686	-0.130446
H	-2.104585	-2.098176	4.216437
H	-2.780569	-2.264204	2.564889
H	-1.434728	-3.339664	3.111297
H	2.448203	2.179995	-0.574674
H	0.896865	1.558810	-1.206630
H	1.414029	2.972359	1.472645
H	-0.243622	4.525880	0.653481
H	-0.316501	3.607114	-0.868762
H	-2.548960	3.036310	0.091797
H	-2.384361	3.513905	2.741208
H	-0.539058	1.762300	3.651502
Ti	-2.565617	-0.169413	-0.905159
Cl	-3.607744	-1.814479	-1.951367
Cl	-3.644184	1.619083	-1.762323
Cl	-0.827451	0.033950	-2.419973
Cl	-3.868328	-0.196863	1.001476

TS **1**

42
scf done: -5309.658553 one negative frequency

C	0.461042	-3.099271	1.370945
C	-0.635894	-2.019823	1.492256
C	0.001346	-0.713730	1.898300
O	1.402368	-1.289725	0.294745
C	1.769975	-2.289668	1.235831
C	-1.436426	-1.624392	0.237098
N	-1.843365	-0.226041	0.554974
C	-0.860929	0.408995	1.440444
C	2.046921	-1.567638	2.547116
C	1.047595	-0.680321	2.854812
P	0.151865	1.771902	0.664042
O	-0.863494	2.725423	-0.097080
C	-0.895664	2.839975	-1.556323
C	-3.076625	0.368466	0.525752
C	-4.200362	-0.298063	-0.341413
Cl	-4.821267	-1.742691	0.562447
O	-3.319341	1.397702	1.135804
O	0.567209	2.520797	2.010169
C	1.720772	3.422532	2.003426
O	1.303126	1.351844	-0.203315
Cl	-5.530865	0.852809	-0.556161
Cl	-3.583344	-0.793783	-1.950252
H	-1.375932	0.911769	2.273516
H	-0.636630	3.871998	-1.793907
H	-0.189200	2.146130	-2.014684
H	-1.919191	2.620055	-1.859441

H	1.828146	3.747702	3.036923
H	2.604681	2.878511	1.667401
H	1.510605	4.277164	1.357328
H	-2.314258	-2.249005	0.087182
H	-0.803985	-1.631490	-0.653772
H	-1.349526	-2.265502	2.294605
H	0.465557	-3.778657	2.229092
H	0.316944	-3.688855	0.460936
H	2.620925	-2.874076	0.880598
H	2.917280	-1.758903	3.162723
H	1.145952	0.118373	3.581279
Ti	2.582633	-0.211145	-0.865880
Cl	3.880461	1.367063	-1.846864
Cl	3.794848	-2.032204	-1.406440
Cl	1.061151	-0.417963	-2.596458
Cl	3.791031	0.118225	1.237079

Complex C**3**

42

scf done: -5309.712257 no negative frequencies

C	-0.447898	3.170459	-0.031828
C	0.637412	2.316710	0.679128
C	0.093953	1.393353	1.749933
O	-2.196632	1.535288	-0.084088
C	-1.869017	2.807321	0.422250
C	1.455782	1.376070	-0.224667
N	1.935715	0.349440	0.727775
C	0.929203	0.129598	1.779074
C	-1.911412	2.768100	1.967930
C	-1.036786	1.628084	2.424153
P	-0.161086	-1.295610	1.319876
O	0.723429	-2.592261	1.026789
C	1.015623	-3.063406	-0.319841
C	3.159213	-0.227728	0.908481
C	4.285769	0.082274	-0.142743
Cl	4.787164	1.813650	0.026482
O	3.408289	-0.966968	1.847685
O	-0.839998	-1.593498	2.731052
C	-1.823204	-2.661452	2.883312
O	-1.075396	-0.980711	0.159999
Cl	5.688687	-0.949360	0.181279
Cl	3.706080	-0.230264	-1.818890
H	1.428453	-0.105309	2.723611
H	0.859463	-4.142238	-0.303538
H	0.352567	-2.588702	-1.045100
H	2.060324	-2.834465	-0.533895
H	-2.115942	-2.630809	3.931631
H	-2.678572	-2.467638	2.234197
H	-1.354081	-3.618626	2.646335

H	2.289900	1.879537	-0.708081
H	0.828074	0.904631	-0.988364
H	1.350913	2.993920	1.170057
H	-0.281372	4.234759	0.167696
H	-0.397351	3.031723	-1.116982
H	-2.598914	3.526627	0.036379
H	-1.600212	3.744145	2.354639
H	-1.418514	0.949156	3.179214
Ti	-2.580112	0.068691	-0.972684
Cl	-4.004585	-1.401897	0.006095
Cl	-4.156736	0.965927	-2.304767
Cl	-1.144341	-0.339074	-2.693052
Cl	-3.605779	2.541291	2.562498

Complex C**2**

43

scf done: -5770.001601 no negative frequencies

C	-1.061370	1.932927	2.532370
C	-0.282647	1.437427	1.340244
C	0.541358	2.605581	0.726089
C	-0.569069	3.515836	0.150954
C	-1.851641	2.706158	0.522018
C	-2.020713	2.717505	2.024841
O	-1.343145	1.341827	0.295401
C	0.691525	0.275212	1.427519
N	1.676677	0.550790	0.358524
C	1.412472	1.864565	-0.292663
C	2.826945	-0.165710	0.395183
O	2.991849	-1.134423	1.124459
P	-0.220777	-1.312439	1.433354
O	-1.350346	-1.385447	0.402968
Ti	-2.438253	-0.271996	-0.854756
Cl	-4.045777	-0.079395	0.812595
O	0.619315	-2.661872	1.356992
C	1.022762	-3.258144	0.093752
O	-0.747417	-1.289753	2.934011
C	-1.866748	-2.127858	3.324612
C	4.003173	0.242086	-0.575425
Cl	3.430773	0.475283	-2.267810
Cl	4.794336	1.744179	0.026686
Cl	5.220598	-1.066703	-0.583132
Cl	-3.434576	-2.040453	-1.826157
Cl	-3.370966	1.389610	-2.116841
Cl	-0.573456	-0.358574	-2.265715
H	1.197606	0.401364	2.419072
H	0.898856	-4.334109	0.222958
H	0.393160	-2.899435	-0.723407
H	2.070314	-3.004569	-0.067591
H	-2.050695	-1.883785	4.370160

H	-2.738033	-1.888790	2.711761
H	-1.591349	-3.180963	3.224679
H	2.350646	2.382573	-0.484130
H	0.882172	1.689423	-1.232616
H	1.152196	3.048225	1.517755
H	-0.574360	4.513099	0.598574
H	-0.493372	3.613476	-0.936990
H	-2.727137	2.871827	-0.098387
H	-2.731875	3.338946	2.555192
H	-0.732598	1.770575	3.550278
Cl	1.976859	1.970847	3.840229

TS **2**

43

scf done: -5769.974506 one negative frequency

C	-0.836047	1.831169	2.629641
C	-0.013633	1.396892	1.535345
C	0.755026	2.457160	0.731041
C	-0.306003	3.422825	0.160074
C	-1.617483	2.775504	0.633825
C	-1.735601	2.752744	2.155585
O	-1.329011	1.364233	0.291503
C	0.838571	0.149200	1.543809
N	1.863752	0.377251	0.513704
C	1.552052	1.611971	-0.268865
C	3.051925	-0.252014	0.721734
O	3.257689	-1.012512	1.657836
P	-0.155311	-1.394004	1.351582
O	-1.394773	-1.318021	0.497094
Ti	-2.518737	0.019811	-0.656411
Cl	-3.995836	0.142213	1.147074
O	0.823068	-2.556015	0.866563
C	0.661096	-3.198468	-0.434445
O	-0.482462	-1.682578	2.891665
C	-1.746524	-2.317701	3.242105
C	4.212595	0.002502	-0.309977
Cl	3.634151	-0.039787	-2.005734
Cl	4.965623	1.611146	0.051458
Cl	5.459055	-1.255839	-0.101641
Cl	-3.633257	-1.776886	-1.549146
Cl	-3.537279	1.646264	-1.861515
Cl	-0.766408	-0.254619	-2.257641
H	1.326636	0.034674	2.520551
H	0.084976	-4.114791	-0.291192
H	0.156539	-2.534486	-1.138609
H	1.672421	-3.429839	-0.769535
H	-1.815221	-2.230671	4.326085
H	-2.571648	-1.795806	2.753450
H	-1.722731	-3.370284	2.948579

H	2.473415	2.093254	-0.592240
H	0.944837	1.334298	-1.134214
H	1.433024	2.966561	1.425874
H	-0.206137	4.434882	0.553703
H	-0.286404	3.418204	-0.934719
H	-2.511966	3.103706	0.111766
H	-2.626082	3.072063	2.671704
H	-0.831846	1.373747	3.610795
Cl	-1.188785	5.196962	2.729344

Complex C**4**

43

scf done: -5770.039493 no negative frequencies

C	-0.832282	1.737080	2.490013
C	0.305335	1.489340	1.829700
C	0.874119	2.376514	0.744197
C	-0.150147	3.326320	0.078249
C	-1.596430	3.014506	0.489460
C	-1.732017	2.830436	2.017719
O	-2.015336	1.832335	-0.111812
C	1.103232	0.198039	1.866663
N	2.075562	0.357002	0.772017
C	1.575029	1.373299	-0.187772
C	3.276436	-0.257542	0.909239
O	3.581517	-0.950128	1.870851
P	-0.080430	-1.171013	1.457996
O	-1.128207	-0.762128	0.477403
Ti	-2.727367	0.243513	-0.622440
Cl	-3.917905	0.163270	1.484888
O	0.761448	-2.434652	0.935373
C	0.541015	-2.959390	-0.409434
O	-0.586157	-1.560676	2.929287
C	-1.795530	-2.371137	3.050087
C	4.338235	-0.052971	-0.237034
Cl	3.642825	-0.384302	-1.859524
Cl	4.961819	1.650812	-0.169545
Cl	5.709685	-1.155945	0.030622
Cl	-3.422503	-1.986800	-1.015759
Cl	-4.438521	1.156173	-1.818893
Cl	-1.187495	0.082962	-2.439871
H	1.627706	-0.032004	2.797913
H	0.617607	-4.043948	-0.317327
H	-0.440949	-2.663393	-0.783771
H	1.328614	-2.575916	-1.060566
H	-1.989803	-2.432434	4.120999
H	-2.620748	-1.880940	2.528226
H	-1.605519	-3.368006	2.643472
H	2.396153	1.821092	-0.743579
H	0.865007	0.911305	-0.884282

H	1.664646	2.981727	1.213865
H	0.075865	4.361370	0.352877
H	-0.092634	3.244800	-1.012195
H	-2.254842	3.832489	0.167200
H	-2.767059	2.606703	2.269675
H	-1.216687	1.055694	3.242833
Cl	-1.386017	4.451464	2.870592

Complex C**5**

41
scf done: -5263.617449 no negative frequencies

C	-0.290783	3.449092	0.541159
C	0.799528	2.406129	0.805806
C	-0.056158	1.170923	1.260359
C	-1.384420	1.259307	0.508267
N	-1.395412	2.633720	-0.030947
C	1.691676	2.625101	2.051950
C	1.178660	1.472530	2.984137
C	1.618307	0.146086	2.379379
C	0.835979	-0.051878	1.309752
O	-0.225775	1.486807	2.653283
P	-2.801255	0.902508	1.650609
O	-2.332959	-0.493299	2.238128
C	-3.158098	-1.256291	3.165894
C	-2.235659	2.873895	-1.071084
C	-2.207235	4.288755	-1.752590
Cl	-3.545257	4.403494	-2.913088
O	-3.012230	2.023824	-1.491744
O	-3.081686	2.052673	2.609716
Fe	-2.640101	2.844789	4.360033
O	-4.131494	0.525788	0.859960
C	-5.224697	1.458661	0.619048
Cl	-2.379365	5.592794	-0.532618
Cl	-0.647936	4.472316	-2.655096
H	-1.453114	0.543173	-0.317083
H	-6.123159	0.843440	0.579378
H	-5.288634	2.179230	1.436126
H	-5.046994	1.948838	-0.337830
H	-2.639301	-2.205388	3.289754
H	-3.214046	-0.725018	4.116891
H	-4.148310	-1.414027	2.733392
H	0.016891	4.216257	-0.165951
H	-0.632923	3.918037	1.467926
H	1.362516	2.197643	-0.108602
H	2.759962	2.554393	1.831976
H	1.487871	3.589993	2.524672
H	1.309393	1.623136	4.053411
H	2.468346	-0.440958	2.706229
H	0.892041	-0.826508	0.554569

Cl	-4.609703	3.517590	5.049283
Cl	-1.854772	1.281539	5.695946
Cl	-1.269214	4.551865	4.116084

TS **3**

41

scf done: -5263.563085 one negative frequency

C	-0.566166	3.434571	0.651192
C	0.550583	2.417458	0.943087
C	-0.184193	1.112919	1.000870
C	-1.471654	1.232255	0.299016
N	-1.487897	2.621925	-0.175236
C	1.455675	2.613699	2.176596
C	1.032081	1.547244	3.194108
C	1.181212	0.152441	2.618363
C	0.460443	-0.063961	1.483086
O	-0.378393	1.660413	3.342404
P	-2.932758	0.919102	1.475891
O	-2.461243	-0.513349	2.008644
C	-3.244366	-1.188056	3.039288
C	-2.173324	2.882537	-1.320520
C	-2.133235	4.343760	-1.888864
Cl	-3.256103	4.469527	-3.254497
O	-2.806754	2.017620	-1.912349
O	-3.169240	2.060543	2.394341
Fe	-1.255193	2.656333	4.747581
O	-4.161511	0.526369	0.520330
C	-5.218900	1.477845	0.217089
Cl	-2.593432	5.533187	-0.631057
Cl	-0.453506	4.679792	-2.485593
H	-1.608552	0.526059	-0.529490
H	-6.150133	0.911215	0.248572
H	-5.232241	2.276983	0.960877
H	-5.041970	1.869912	-0.785166
H	-2.699495	-2.105791	3.257422
H	-3.304265	-0.554123	3.925614
H	-4.236509	-1.420847	2.645355
H	-0.206613	4.301623	0.102566
H	-1.071423	3.750037	1.569510
H	1.167363	2.329874	0.031022
H	2.518342	2.542162	1.921248
H	1.271367	3.600588	2.615145
H	1.546398	1.667228	4.151037
H	1.658367	-0.652447	3.170187
H	0.226615	-1.047791	1.090025
Cl	-2.867765	1.496253	5.719435
Cl	0.413145	2.856426	6.210077
Cl	-1.724281	4.699430	4.029282

Complex C**6**

41
scf done: -5263.598445 no negative frequencies

C	-1.031751	3.493623	0.355761
C	0.040838	2.728479	1.149228
C	-0.567561	1.345816	1.310393
C	-1.688513	1.178072	0.309369
N	-1.618697	2.425955	-0.478202
C	0.440164	3.332601	2.504828
C	1.244682	2.314841	3.303457
C	0.937487	0.881328	3.149789
C	-0.157400	0.476257	2.245994
O	0.482700	1.640471	4.368765
P	-3.344981	1.105061	1.154292
O	-3.137836	-0.247182	2.001135
C	-4.186373	-0.675055	2.907177
C	-1.948430	2.371218	-1.795743
C	-1.778089	3.676749	-2.656113
Cl	-2.413357	3.392138	-4.285220
O	-2.366597	1.355359	-2.333496
O	-3.677830	2.367092	1.874018
Fe	1.220501	1.297819	6.246769
O	-4.425423	0.624853	0.058452
C	-5.280739	1.573394	-0.624639
Cl	-2.674809	5.051663	-1.913882
Cl	-0.018202	4.081395	-2.784306
H	-1.582129	0.317105	-0.356630
H	-6.255798	1.093333	-0.719137
H	-5.367446	2.494640	-0.043949
H	-4.859642	1.766896	-1.612985
H	-3.769951	-1.509853	3.469979
H	-4.453576	0.140988	3.582683
H	-5.056722	-1.000258	2.331880
H	-0.618688	4.293468	-0.253364
H	-1.810868	3.889240	1.016019
H	0.931308	2.638080	0.509373
H	1.025423	4.248150	2.372940
H	-0.460602	3.586000	3.074155
H	2.244522	2.586280	3.631616
H	1.703332	0.157084	3.414229
H	-0.611014	-0.500293	2.376324
Cl	0.024061	-0.381095	6.939171
Cl	3.305711	0.805106	5.757404
Cl	0.952773	3.224149	7.218951

TS **4**

41
-5263.57548839 one negative frequency

C	1.5512	1.4072	4.7289

C	0.7675	1.3817	3.5893
C	0.8138	2.4867	2.5737
C	0.9206	3.8566	3.2668
C	2.0895	3.8657	4.2745
C	2.3265	2.5444	4.9409
C	-0.4148	2.2186	1.6855
N	-0.5480	0.7528	1.7965
C	-0.1814	0.3338	3.1503
O	1.7387	4.6673	5.3696
Fe	2.2344	4.6697	7.1919
Cl	4.4371	4.3742	7.1947
P	-1.7623	0.2852	4.2370
O	-2.8771	1.0094	3.5713
C	-1.1127	-0.1835	0.9890
C	-1.5165	0.2373	-0.4647
Cl	-2.7387	1.5512	-0.4080
O	-2.0205	-1.2553	4.6104
C	-3.0444	-2.0264	3.9178
O	-1.1348	0.8604	5.5891
C	-1.9425	1.0007	6.7955
O	-1.2677	-1.3408	1.3576
Cl	1.5167	6.5058	8.1374
Cl	1.2976	2.7853	8.0071
Cl	-0.0414	0.8002	-1.3509
Cl	-2.1955	-1.1599	-1.3129
H	0.2193	-0.6851	3.1597
H	-3.2267	-2.8916	4.5547
H	-3.9499	-1.4268	3.8091
H	-2.6656	-2.3304	2.9417
H	-1.3032	1.5262	7.5027
H	-2.8357	1.5873	6.5709
H	-2.2092	0.0089	7.1660
H	-0.2636	2.5247	0.6527
H	-1.3164	2.6960	2.0861
H	1.7187	2.3110	1.9692
H	1.0388	4.6587	2.5325
H	0.0042	4.0459	3.8348
H	3.0194	4.2200	3.8005
H	3.1057	2.5436	5.7014
H	1.5785	0.5770	5.4257

Complex C**7**

41

-5263.59330413 no negative frequencies

C	2.7055	1.4596	4.2805
C	1.6149	1.3503	3.5027
C	1.1961	2.3939	2.4915
C	1.7421	3.7777	2.8456
C	3.2577	3.6475	3.0636

C	3.5726	2.6557	4.1948
C	-0.3259	2.1954	2.4243
N	-0.4297	0.7246	2.5423
C	0.5783	0.2450	3.5129
O	3.8529	4.8936	3.2732
Fe	4.6294	5.5081	4.8068
Cl	6.7026	4.8661	5.0889
P	-0.2482	0.0791	5.1699
O	-0.9946	1.3019	5.5774
C	-1.0857	-0.2039	1.7952
C	-2.0863	0.3057	0.6938
Cl	-3.2789	1.4583	1.3950
Cl	3.3597	3.6560	5.8574
O	-1.1125	-1.2801	5.1314
C	-2.5466	-1.2581	4.9284
O	1.0239	-0.3912	6.0426
C	0.8307	-0.6892	7.4480
O	-0.9365	-1.4077	1.9501
Cl	3.9775	7.4336	5.5775
Cl	-1.1509	1.1099	-0.6315
Cl	-2.9589	-1.0770	0.0105
H	0.9504	-0.7349	3.1983
H	-2.9713	-1.9707	5.6372
H	-2.9426	-0.2574	5.1156
H	-2.7496	-1.5785	3.9052
H	1.8242	-0.8870	7.8496
H	0.3811	0.1682	7.9548
H	0.1972	-1.5734	7.5522
H	-0.7621	2.5544	1.4960
H	-0.8338	2.6532	3.2795
H	1.6007	2.0890	1.5119
H	1.5622	4.4996	2.0435
H	1.2751	4.1594	3.7612
H	3.7076	3.1933	2.1628
H	4.6409	2.4427	4.2623
H	2.9612	0.6970	5.0086

TS **5**

41

-5263.57105927 one negative frequency

C	-1.0813	3.4974	0.4110
C	-0.0809	2.7126	1.2754
C	-0.6889	1.3388	1.3643
C	-1.7286	1.1757	0.2967
N	-1.6232	2.4359	-0.4632
C	0.2757	3.2761	2.6550
C	1.0774	2.2480	3.4483
C	0.6834	0.8642	3.2826
C	-0.2564	0.4408	2.2868

O	1.6950	2.6929	4.5248
P	-3.4324	1.0625	1.0677
O	-3.1951	-0.2460	1.9691
C	-4.2512	-0.6889	2.8634
C	-1.9146	2.4027	-1.7921
C	-1.7203	3.7196	-2.6257
Cl	-2.2953	3.4567	-4.2790
O	-2.3155	1.3918	-2.3519
O	-3.8351	2.3378	1.7221
Fe	1.7083	1.7517	6.2169
O	-4.4311	0.5002	-0.0591
C	-5.3005	1.3839	-0.8134
Cl	-2.6501	5.0732	-1.8881
Cl	0.0408	4.1331	-2.6822
H	-1.5837	0.3200	-0.3700
H	-6.2375	0.8427	-0.9486
H	-5.4726	2.3097	-0.2599
H	-4.8335	1.5802	-1.7797
H	-3.8105	-1.4770	3.4725
H	-4.5768	0.1408	3.4946
H	-5.0850	-1.0807	2.2762
H	-0.6108	4.2874	-0.1686
H	-1.8940	3.9094	1.0180
H	0.8575	2.5978	0.6992
H	0.8496	4.2029	2.5750
H	-0.6278	3.4815	3.2444
H	1.8727	1.6938	2.6754
H	1.1859	0.1377	3.9184
H	-0.6051	-0.5853	2.3112
Cl	-0.3905	0.9905	6.1978
Cl	3.0722	0.0362	5.9121
Cl	2.2282	3.1278	7.8207

Complex C**8**

41

-5263.63560772 no negative frequencies

C	-1.1958	3.5088	0.5472
C	-0.2116	2.7632	1.4658
C	-0.7357	1.3403	1.4705
C	-1.6918	1.1593	0.3093
N	-1.5932	2.4509	-0.4021
C	-0.1283	3.2951	2.9039
C	0.6433	2.3402	3.7740
C	0.4836	0.8551	3.5742
C	-0.4328	0.4728	2.4411
O	1.3868	2.8018	4.6598
P	-3.4301	0.9615	0.9279
O	-3.2928	-0.4840	1.6276
C	-4.4652	-1.0806	2.2344

C	-1.7690	2.4560	-1.7514
C	-1.5872	3.8190	-2.5156
Cl	-2.0127	3.5977	-4.2202
O	-2.0580	1.4527	-2.3868
O	-3.8768	2.1219	1.7533
Fe	2.5449	1.9072	6.0884
O	-4.3732	0.6076	-0.3308
C	-5.1931	1.6152	-0.9698
Cl	-2.6574	5.0881	-1.8096
Cl	0.1417	4.3402	-2.4119
H	-1.4431	0.3454	-0.3768
H	-6.1521	1.1420	-1.1865
H	-5.3352	2.4699	-0.3046
H	-4.7052	1.9149	-1.8991
H	-4.1168	-1.9888	2.7256
H	-4.8988	-0.3961	2.9679
H	-5.1958	-1.3253	1.4596
H	-0.7411	4.3530	0.0352
H	-2.0823	3.8387	1.0997
H	0.7844	2.7893	1.0006
H	0.3113	4.2927	2.9852
H	-1.1501	3.3307	3.3163
H	1.4979	0.4386	3.4516
H	0.1382	0.4393	4.5335
H	-0.8458	-0.5307	2.4527
Cl	1.0904	0.7007	7.1953
Cl	3.9402	0.7171	4.8927
Cl	3.4272	3.5547	7.1902

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