

Iron(III)Porphyrin Electrocatalyzed Enantioselective Carbon-Chloride Bond Cleavage of Hexachlorocyclohexanes (HCHs): A Combined Experimental Investigation and Theoretical Calculation

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Supplementary Information

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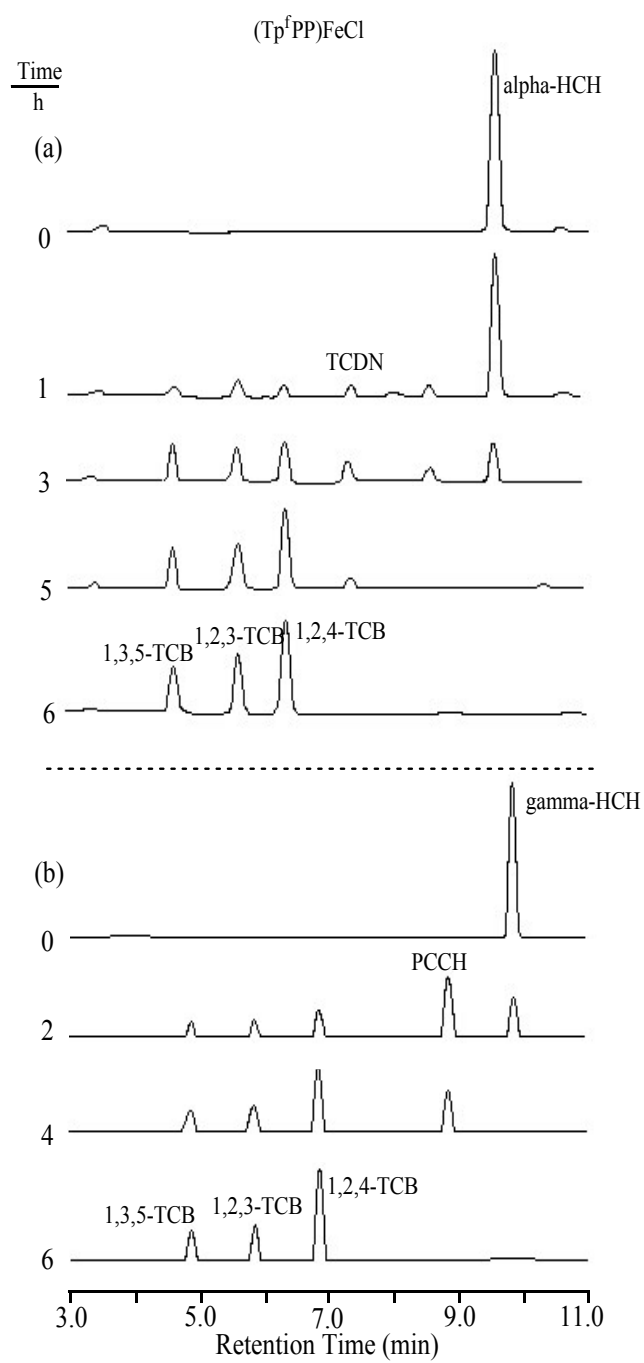


Figure S1. Retention times observed during the GC-MS analyses.

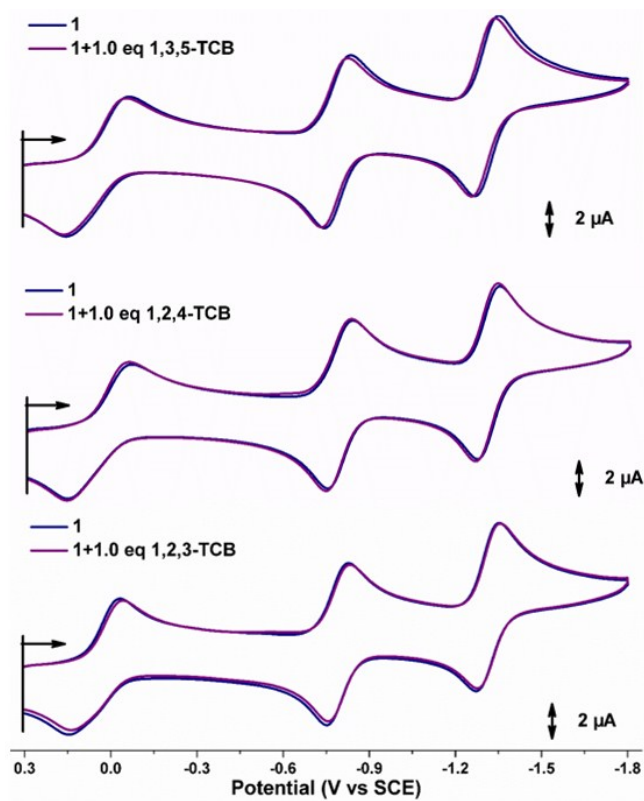


Figure S2 Reductive electrochemical measurements for **1** in the absence (black) and/or presence 1.0 eq of 1,3,5-, 1,2,4- and 1,2,3-trichlorobenzene (TCB) in DMF containing 0.1 M TBAP.

Summary of Computational Data

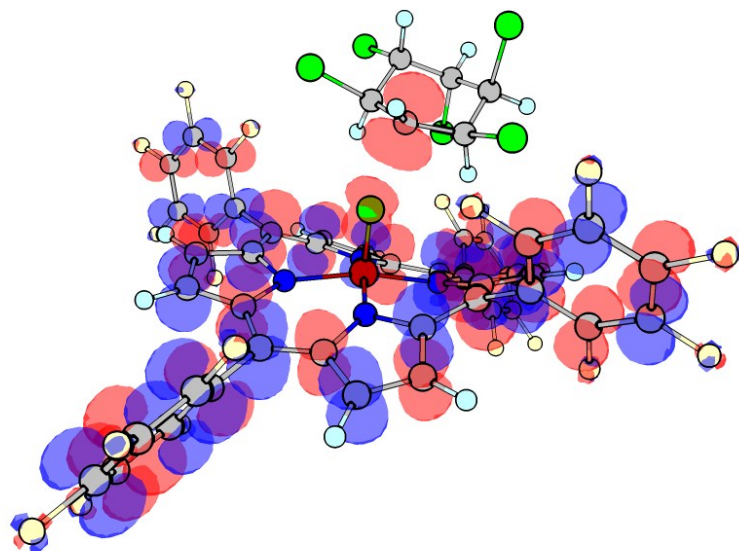
Table S1. Summary of computational data for the transition states that were identified.

Filename	G (Ha)	E (Ha)	Low Freq (cm ⁻¹)	N _{imag}	Comment
alphaa	-0.04647	-0.11218	48.49	0	Most stable conformation
alphab	-0.04635	-0.11097	18.19	0	
betaa	-0.04236	-0.10698	36.50	0	Most stable conformation
betab	-0.0415	-0.10787	41.19	0	
deltaa	-0.03998	-0.10623	46.46	0	
deltab	-0.04177	-0.10691	39.17	0	Most stable conformation
gamma	-0.04428	-0.11045	53.48	0	Only one conformation possible
porph2	-0.83552	-1.15018	5.95	0	porphyrin
alphab_b_full_ts	-0.85741	-1.26177	-631.64	1	Cl transfer TS
alphab_c_full_ts	-0.77286	-1.18759	-846.67	1	Cl transfer TS
deltaa_a_full_ts	-0.84644	-1.25407	-650.96	1	Cl transfer TS
deltaa_b_full_ts	-0.85137	-1.26147	-490.60	1	Cl transfer TS
deltaa_c_full_ts	-0.82707	-1.23371	-665.04	1	Cl transfer TS
deltaa_d_full_ts	-0.83069	-1.2373	-571.49	1	Cl transfer TS
deltab_a_full_ts	-0.8307	-1.23689	-659.38	1	Cl transfer TS
deltab_d_full_ts	-0.84107	-1.24996	-577.08	1	Cl transfer TS
gammaa_b_full_ts	-0.84186	-1.24998	-585.26	1	Cl transfer TS
alphaa_2_1_ts	-0.86896	-1.27654	-90.51	1	Cl abstraction TS
alphab_1_1_ts	-0.85336	-1.25695	-91.83	1	Cl abstraction TS
betaaa_1_ts	-0.88472	-1.28707	-117.19	1	Cl abstraction TS
deltab_1_ts	-0.88401	-1.28843	-101.58	1	Cl abstraction TS
deltab_2_ts	-0.86491	-1.27219	-101.12	1	Cl abstraction TS
deltab_3_ts	-0.88277	-1.28612	-103.79	1	Cl abstraction TS
gamma_1_ts	-0.88847	-1.29077	-76.55	1	Cl abstraction TS
gamma_2_ts	-0.87238	-1.27765	-109.43	1	Cl abstraction TS
gamma_3_ts	-0.87733	-1.28167	-103.49	1	Cl abstraction TS

XYZ Coordinates of Structures

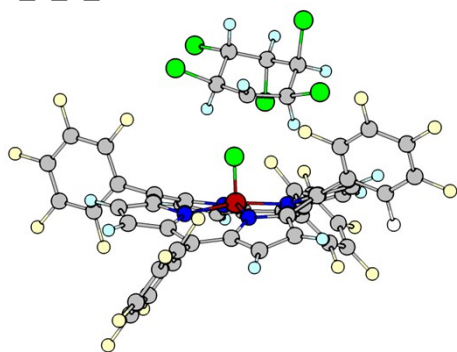
Cl Abstraction Spin Density at Transition state

alphaa_2_1_ts



Cl Abstraction Transition States

alphaa_2_1_ts

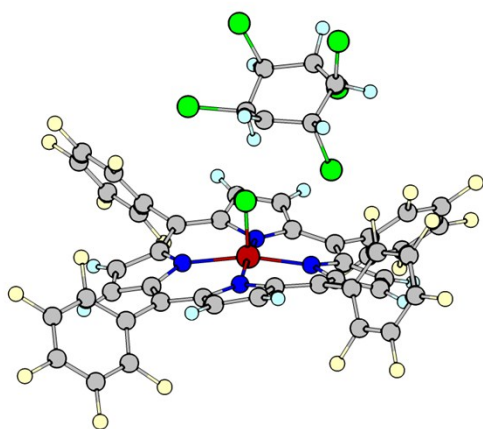


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C	3.58622	1.60259	-0.50504
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C	-0.86115	2.73604	-1.06036

N	-1.11368	1.36821	-0.71292
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C	0.68361	4.65778	-1.49046
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H	3.24216	3.76220	-0.84636
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H	-4.83474	-2.15908	0.04161
Fe	-0.12697	-0.31262	-0.61457
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F	1.96645	4.18915	-3.43580
F	2.42351	6.79816	-3.94058
F	1.37537	8.73727	-2.29800
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alphan_1_1_ts

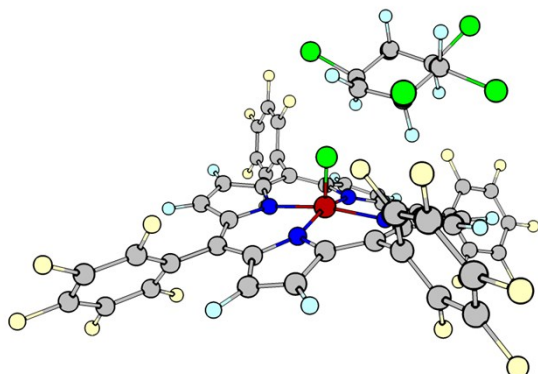


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betaaa_1_ts

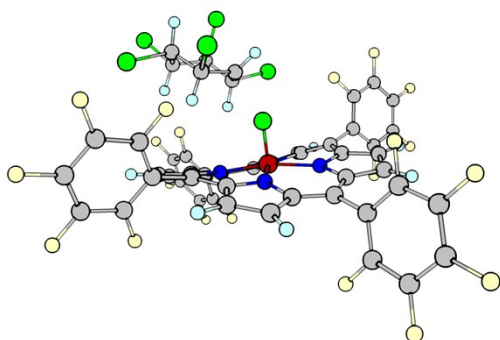


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C	4.85663	-1.98158	0.74324
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C	7.19819	-1.90302	0.09566
C	6.83675	-1.19296	-1.05853
C	5.48681	-0.88384	-1.29778
H	3.76306	-3.42856	-1.70422
H	1.64678	-4.94854	-2.41554
H	3.25406	3.70038	-0.44781
H	4.61930	1.41544	-0.07781
H	-2.10720	4.56708	-1.23481
H	-4.16685	2.92360	-0.71147
H	-4.96745	-2.13425	-0.26013
Fe	-0.17865	-0.34443	-0.59157
H	-3.63066	-4.29647	-1.18344
F	1.82180	4.22529	-3.22730
F	2.32771	6.85056	-3.63608
F	1.47937	8.71498	-1.82598
F	0.14253	7.90870	0.41954
F	-0.31834	5.28290	0.86031
F	-4.15080	0.50832	2.43105
F	-6.69294	0.98433	3.24295
F	-8.70074	1.20831	1.40273
F	-8.13452	0.94939	-1.25748
F	-5.59282	0.47320	-2.06750
F	-2.57838	-4.35623	-3.84771
F	-3.10823	-6.86551	-4.68051
F	-1.93878	-9.02145	-3.43479
F	-0.27459	-8.59172	-1.28671
F	0.19892	-6.08928	-0.40716
F	3.93862	-2.37926	1.61398
F	6.53549	-2.97939	2.09257
F	8.47322	-2.19762	0.33002
F	7.77498	-0.82055	-1.92512
F	5.17971	-0.23360	-2.41304
C	1.93691	1.99734	4.09994
C	0.72379	2.92680	4.20114
C	-0.54034	2.14778	4.57636
C	-0.82436	1.01903	3.56641
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Cl	3.33061	2.97913	3.54360
H	2.21225	1.58999	5.10546
Cl	1.04701	4.11581	5.51269
H	0.57834	3.51600	3.25762

H	-0.46671	1.74179	5.61663
Cl	-1.91529	3.29805	4.56758
Cl	-2.09213	-0.03773	4.30823
H	-1.28269	1.43823	2.63027
H	0.37762	-0.83928	3.63619
Cl	-0.09338	-0.48577	1.07398
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deltab_1_ts

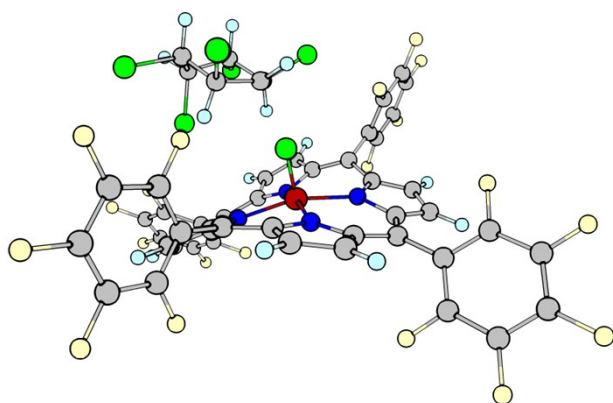


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C	0.52353	-3.40120	-1.43692
C	3.07548	2.53255	-1.29926
C	3.77519	1.35496	-1.13340
C	2.80003	0.29765	-0.92433
N	1.48352	0.82564	-0.91773
C	1.68114	2.22263	-1.14293
C	-1.75077	3.55999	-0.31316
C	-0.63138	2.72843	-0.64937
N	-0.95922	1.34545	-0.52038
C	-2.32737	1.35735	-0.14453
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C	0.94168	4.59598	-1.17108
C	4.58924	-1.34134	-0.50496
C	-1.15717	-5.11270	-2.12085
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C	1.64189	6.50465	-2.57071
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C	-7.22151	0.82651	1.38959
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C	5.53255	-1.54509	-1.53245
H	3.80141	-3.77847	-1.25243
H	1.65724	-5.27344	-1.86912
H	3.45784	3.51932	-1.48313
H	4.83385	1.21471	-1.16481
H	-1.74538	4.63330	-0.35639
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Fe	-0.01076	-0.38878	-0.59141
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C	1.04939	2.69943	3.86347
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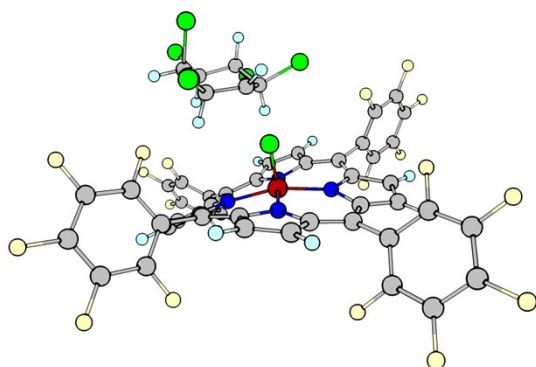


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C	3.01295	-0.82890	-0.55657
C	-0.82051	-3.68729	-1.76715
C	0.64745	4.65194	-1.57205
C	4.30412	-1.25782	-0.02360
C	-1.12833	-4.98027	-2.34939
C	-4.62137	0.42866	0.49330
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C	1.08581	7.43210	-2.19738
C	0.34695	7.05365	-1.05201
C	0.15308	5.71716	-0.75275
C	-4.88328	0.32937	1.87525
C	-6.17310	0.49878	2.40747
C	-7.25025	0.77251	1.55374
C	-7.02611	0.86751	0.17287
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C	-2.06982	-5.12005	-3.40378
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C	-1.74406	-7.52974	-3.51393
C	-0.81277	-7.43174	-2.46743
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C	6.79817	-2.12944	1.08104
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H	3.79367	-3.16866	-1.98856
H	1.74209	-4.73234	-2.73983
H	3.19964	3.78717	-0.83805
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Fe	-0.13830	-0.30005	-0.61296
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Cl	0.30613	3.48222	2.35296
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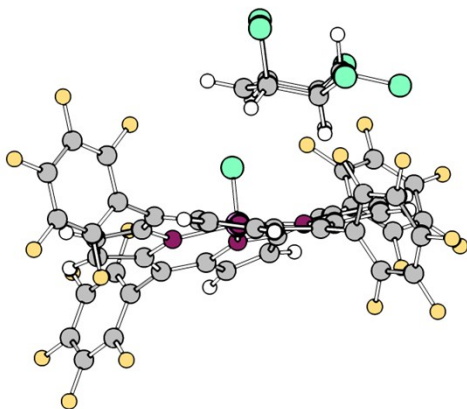


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C	-2.99705	-1.10500	-0.48277
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C	-1.89208	-2.92449	-1.17327
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C	0.70815	4.65356	-1.04977
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C	-4.79816	0.48138	0.09557
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C	0.49883	6.99630	-0.29275
C	0.25944	5.62234	-0.12199
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C	-6.46375	1.17020	1.77774
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H	3.26179	3.69055	-0.37563
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Fe	-0.17250	-0.35568	-0.57197
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F	6.59221	-2.93851	2.02191
F	8.49296	-2.20590	0.19965
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F	5.14918	-0.27058	-2.50359
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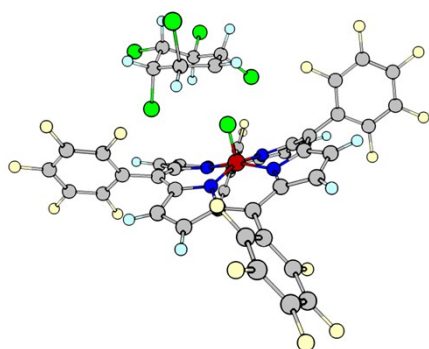
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H	1.19841	-5.07872	-1.09982
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Fe	-0.34017	-0.15984	-0.58869
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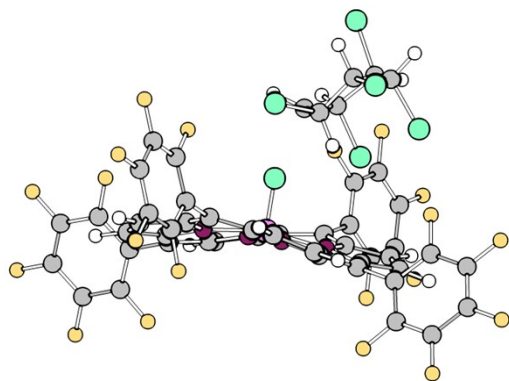


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C	0.11888	4.82667	1.45142
C	-5.94337	1.70646	-1.27716
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C	-1.06357	-4.93354	1.44834
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C	6.66605	-2.18182	-2.13989
C	7.08449	-1.56154	-3.32722
C	6.21029	-0.68341	-3.98642
C	4.92919	-0.44366	-3.46319
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H	3.27876	3.49192	-0.06697
H	4.73304	1.51238	-1.19679
H	-1.66007	4.77219	-0.86957
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Fe	-0.24350	-0.15007	-0.66314
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F	-0.19753	6.43067	3.15485
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F	-1.17887	-6.44004	3.27945
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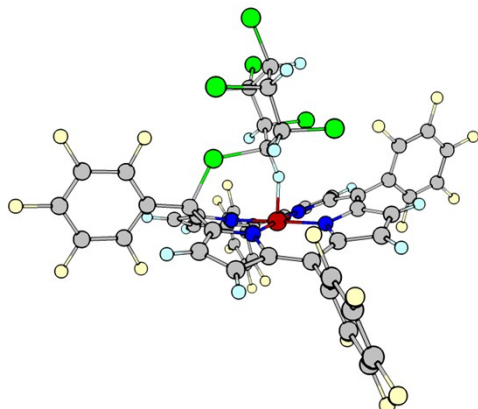
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C	7.31047	-1.87532	0.06364
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Cl Transfer Mechanism

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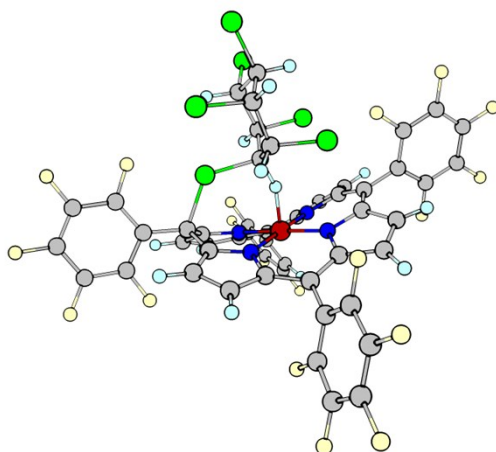


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C	1.59190	7.01469	-1.69320
C	1.93680	7.16432	-3.04409
C	1.94230	6.04060	-3.88255
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F	1.58835	8.07585	-0.89104
F	2.25623	8.36169	-3.52546
F	2.26905	6.17553	-5.16485
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F	3.78633	-1.57917	2.50920
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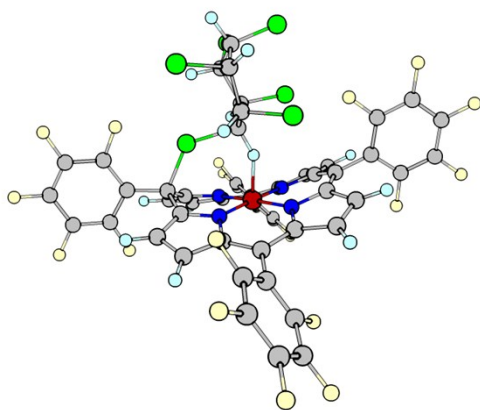


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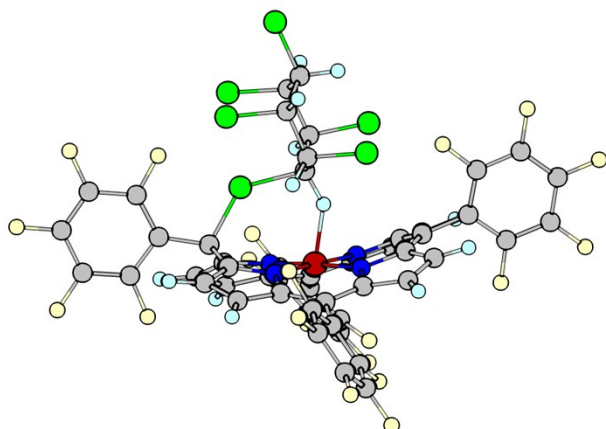
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C	-7.17230	-1.16747	-1.84610
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C	1.47073	-6.08041	1.98071
C	1.85285	-7.05457	1.04874
C	1.88027	-6.73017	-0.31496

C	1.52748	-5.43589	-0.73223
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C	6.76890	2.46794	-2.09082
C	7.22340	1.80837	-3.25726
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F	5.19005	2.73898	-0.39726
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C	-0.09370	0.13317	1.97374
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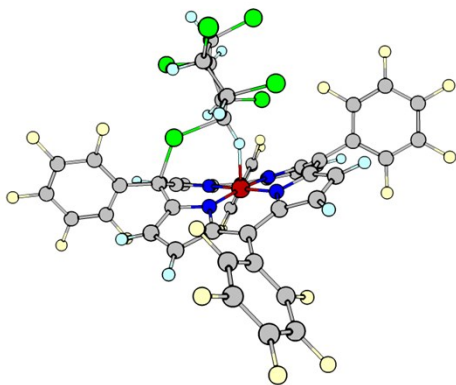


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C	3.61428	0.31866	-1.41101
C	0.63313	-3.23617	0.13599
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H	-3.09435	3.84168	-1.32426
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Fe	0.13097	-0.14046	-0.83626
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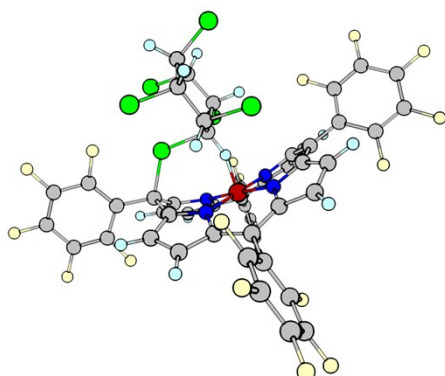


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C	5.82552	-0.39652	-1.51452
C	7.13159	-0.33470	-1.96871
C	7.46367	0.46441	-3.09009
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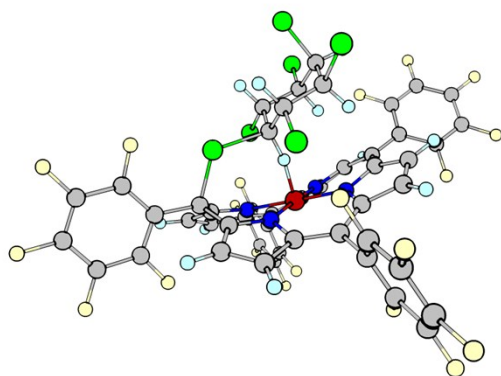


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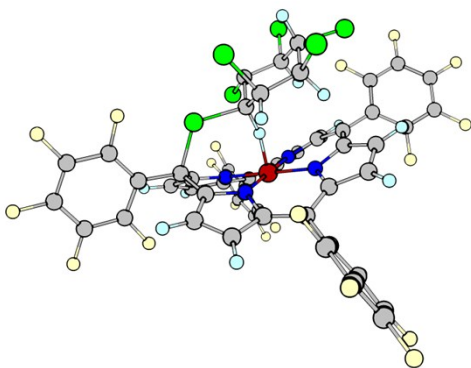


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H	2.30654	-1.72623	1.79701
C	0.04206	-4.33751	-2.19213
C	-4.81289	-0.33998	1.03218
C	-0.68885	4.65091	-1.85289
C	4.72372	0.50137	-0.06284
C	5.25250	1.23379	1.04865
C	6.60665	1.31201	1.32721
C	7.55320	0.68489	0.48142
C	7.07560	0.00862	-0.66990
C	5.71870	-0.06309	-0.92485
C	-0.86991	5.81009	-1.07069
C	-1.02536	7.08142	-1.64957
C	-0.99573	7.22273	-3.04416

C	-0.80898	6.08910	-3.84752
C	-0.65735	4.82474	-3.25178
C	-5.75714	-0.23811	-0.02322
C	-7.14020	-0.34777	0.18063
C	-7.64135	-0.56675	1.47228
C	-6.74045	-0.67173	2.53354
C	-5.35086	-0.55908	2.30944
C	0.29726	-4.51481	-3.56570
C	0.36030	-5.79306	-4.14922
C	0.16985	-6.93344	-3.35678
C	-0.08017	-6.78734	-1.98405
C	-0.13838	-5.50339	-1.41723
F	4.41275	1.84171	1.88953
F	7.03919	1.97947	2.40036
F	8.85441	0.74034	0.75047
F	7.95647	-0.53206	-1.51685
F	5.32834	-0.61903	-2.07354
F	-0.88796	5.71257	0.25197
F	-1.19797	8.15354	-0.88098
F	-1.14280	8.42174	-3.59974
F	-0.77873	6.21634	-5.17139
F	-0.48465	3.77188	-4.03880
F	-5.34343	-0.03210	-1.26594
F	-7.98097	-0.24497	-0.84531
F	-8.94948	-0.67238	1.67984
F	-7.19281	-0.87969	3.76766
F	-4.59496	-0.67562	3.39282
F	0.47767	-3.45446	-4.34101
F	0.59737	-5.92616	-5.45139
F	0.22529	-8.14499	-3.90171
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F	-0.36340	-5.39054	-0.11453

deltab_d_full_ts

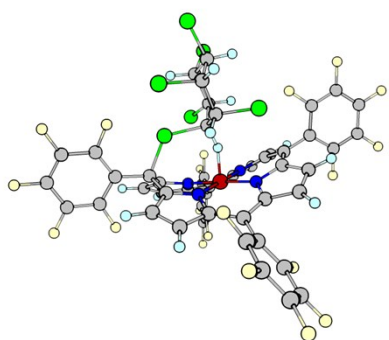


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C	2.73083	-1.53320	0.06181
C	-3.39554	-2.01542	0.44960
C	-2.56488	-3.02123	0.93569
C	-1.27184	-2.43913	1.12460
N	-1.27983	-1.08813	0.73843
C	-2.61727	-0.81713	0.39089
C	-2.75567	2.97198	0.66631
C	-2.26653	1.63536	0.38957
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C	-0.53075	2.84851	1.10703
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N	1.79975	1.22382	0.41881
C	3.06278	0.91141	-0.06610
C	3.97738	1.98691	0.14375
C	0.79104	3.27167	1.35443
C	-3.10238	0.51382	0.17278
C	-0.10200	-3.14534	1.53097
C	3.31527	-0.39964	-0.69284
H	2.54339	-4.43966	1.61416
H	4.34910	-3.05191	0.20958
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Fe	0.26728	0.04915	0.57155
H	5.00320	2.00535	-0.14812
C	-0.28715	-4.40697	2.24635
C	4.77237	-0.61711	-1.03133
C	1.00181	4.58826	1.97523
C	-4.52727	0.72792	-0.04469
C	5.70322	-0.66268	0.04135
C	7.07867	-0.85403	-0.15197
C	7.58811	-1.01207	-1.44914
C	6.70194	-0.97533	-2.52615
C	5.31928	-0.78182	-2.31264
F	5.28606	-0.52279	1.29204
F	7.90615	-0.88701	0.88987
F	8.89009	-1.19350	-1.64631
F	7.16145	-1.12379	-3.76663
F	4.58049	-0.76835	-3.41432
C	1.42117	5.71166	1.23079
C	1.63742	6.96462	1.83001
C	1.42634	7.12789	3.20661
C	0.99751	6.03340	3.97122
C	0.78988	4.78630	3.35673
F	1.60455	5.60121	-0.07828
F	2.03596	8.00076	1.09657

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F	0.38829	3.77157	4.10956
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C	-5.49687	0.25566	0.88349
F	-4.23944	1.97360	-2.05985
F	-6.87015	2.25619	-2.44076
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F	-0.81522	-7.98523	4.36478
F	-1.51315	-5.59995	5.50225
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gammaa_b_full_ts



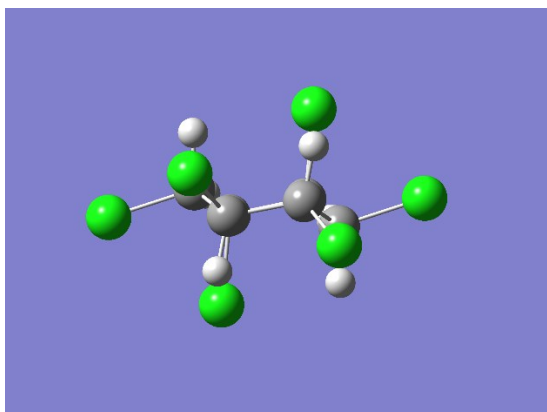
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N	1.56944	1.28873	-0.72335
C	1.62422	2.62130	-1.15299
C	2.96294	3.15375	-0.98071
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C	-3.03499	2.82779	-0.76390
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H	4.74715	2.19080	-0.11565
H	3.26848	4.14159	-1.24545
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Fe	0.06447	0.05489	-0.78300
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C	7.31222	-0.89913	1.49124

C	7.08254	-0.78841	0.11236
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F	6.43821	-0.92694	3.68634
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F	1.01932	8.40977	-3.98678
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F	1.18254	5.68577	-0.14172
C	-5.40650	0.77877	-0.63593
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F	-7.07573	0.29538	3.08186
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C	-1.18210	-5.56990	-1.93603
F	1.18219	-3.86479	-4.11056
F	1.01098	-6.23940	-5.36299
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F	-2.05393	-7.76217	-2.08637
F	-1.79246	-5.44208	-0.75777
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C	0.44665	0.91788	2.82206
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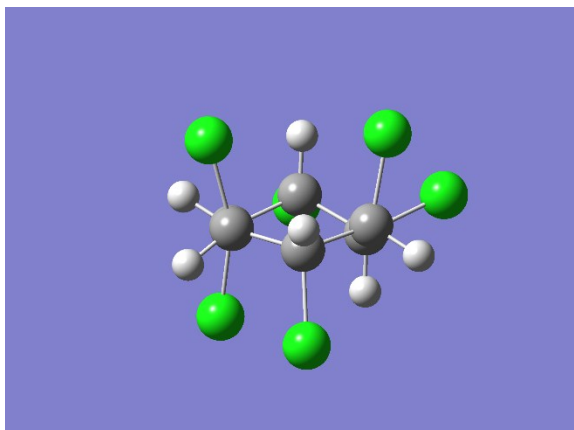
Minima

alphaa



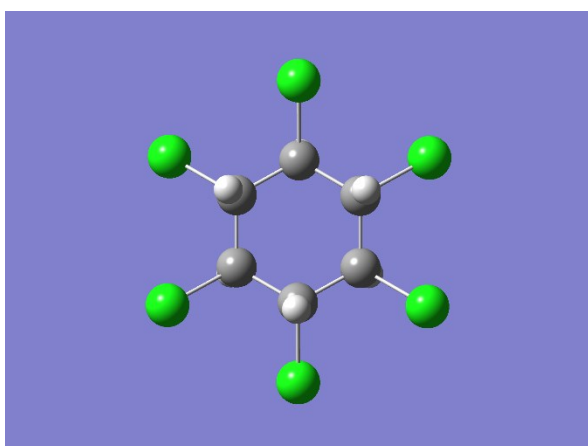
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C	-2.15183	-1.46130	-0.21485
C	-3.66360	-1.63996	-0.02365
H	-5.55750	-0.61382	-0.41312
Cl	-4.23911	-0.39943	-2.37342
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alphan



C	-4.31972	-0.50873	-0.65806
C	-3.90120	0.80996	-0.00570
C	-2.85753	0.57050	1.08907
C	-1.64471	-0.22040	0.58497
C	-1.94219	-1.38411	-0.36935
C	-3.12316	-1.19057	-1.32770
H	-4.78245	-1.20037	0.09888
Cl	-5.55329	-0.18950	-1.90152
H	-3.49598	1.52525	-0.77355
Cl	-5.32429	1.58328	0.73363
H	-2.53141	1.55479	1.52354
Cl	-3.60409	-0.33426	2.43955
Cl	-0.58440	0.94874	-0.27608
H	-1.04143	-0.59161	1.45982
H	-1.01543	-1.64214	-0.95385
Cl	-2.31196	-2.83725	0.62274
Cl	-2.57275	-0.20514	-2.71541
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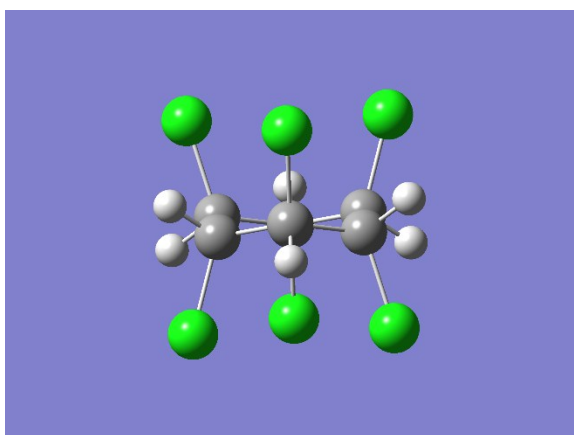
betaa



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C	-2.15432	-1.45478	-0.22349
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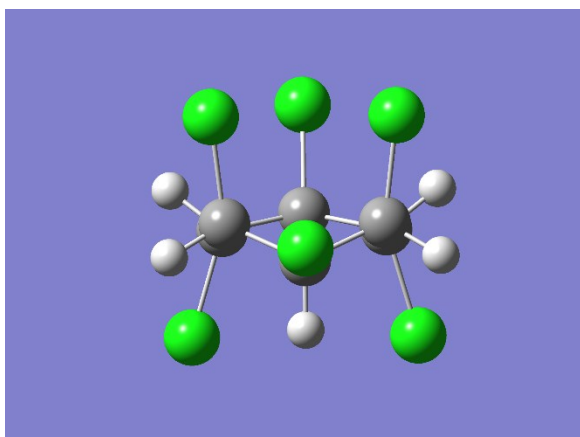
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H	-2.22646	1.24593	-1.30515
Cl	-1.99061	2.54088	0.66595
Cl	0.03567	0.10629	-0.14784
H	-1.69341	-0.11223	1.45848
H	-1.86938	-1.56453	-1.30309
Cl	-1.31752	-2.75650	0.66983
Cl	-4.14983	-3.11755	-0.92482
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betab



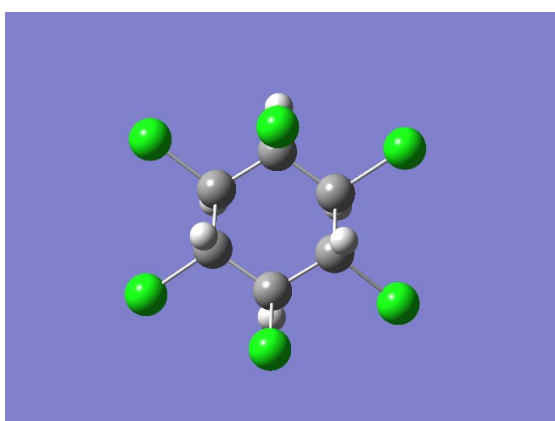
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C	-2.19219	-1.42088	-0.32087
C	-3.59706	-1.52831	0.27461
Cl	-3.79058	-0.17238	2.60018
H	-5.34250	-0.35337	0.84639
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H	-3.97759	1.90992	0.95308
H	-2.41060	1.99187	-1.17641
Cl	-1.31875	1.80486	0.89480
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H	-0.67438	0.00804	-0.95994
H	-2.03931	-2.25525	-1.06664
Cl	-1.00572	-1.77580	0.98735
Cl	-4.69814	-2.15018	-1.00836
H	-3.60629	-2.33720	1.06285

deltaa



C	-3.77347	3.67626	-1.21295
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C	-2.35708	2.07402	0.30622
C	-3.64028	1.30383	0.63922
C	-4.67230	1.43000	-0.47923
C	-5.02473	2.86993	-0.84569
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Cl	-3.36823	3.23190	-2.91539
H	-1.60291	3.66655	-0.98211
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H	-3.40658	0.21432	0.80468
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H	-4.26297	0.91896	-1.39985
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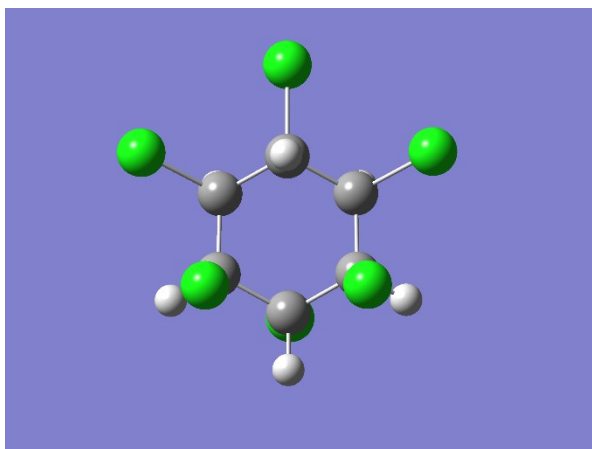
deltab



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C	-2.36700	1.32285	0.08790
C	-3.68051	0.63542	-0.30646
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H	-3.60583	3.69932	1.38236

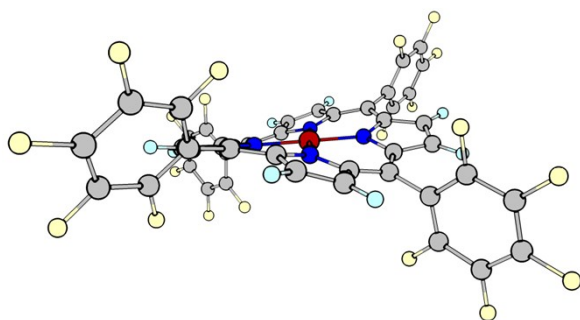
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H	-2.13540	1.14453	1.17301
H	-3.79202	0.59850	-1.42181
Cl	-3.65672	-1.05221	0.26173
H	-5.84126	0.81247	0.05335
Cl	-4.75063	1.27248	2.10007
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Cl	-6.32801	3.58902	0.64206

gamma



C	-4.47072	-0.46666	-0.54019
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C	-2.45666	1.05754	-0.23681
C	-1.67476	-0.11073	0.37732
C	-2.13949	-1.43825	-0.23514
C	-3.64508	-1.66106	-0.05150
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H	-4.50583	1.72556	-0.59003
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H	-2.21722	1.16227	-1.32936
Cl	-1.96064	2.57600	0.55023
Cl	0.05409	0.10872	-0.01218
H	-1.77237	-0.12239	1.49640
H	-1.88128	-1.48120	-1.32759
Cl	-1.27956	-2.78333	0.55381
H	-3.95637	-2.59805	-0.58714
Cl	-4.00807	-1.92414	1.67455

porph2



N	1.12315	-1.58135	-1.02433
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C	1.75739	-3.82882	-0.85667
C	0.69455	-2.87374	-0.69394
C	2.81972	2.86108	-0.97573
C	3.63015	1.84243	-1.43015
C	2.81211	0.65629	-1.47892
N	1.46871	0.93365	-1.10091
C	1.48770	2.31226	-0.80547
C	-2.06560	3.70257	-0.82307
C	-0.95495	2.74282	-0.73979
N	-1.38803	1.44286	-1.02476
C	-2.77259	1.59454	-1.29832
C	-3.16658	3.00268	-1.20754
C	-3.95119	-1.96351	-1.01470
C	-3.15077	-0.77573	-1.16199
N	-1.78015	-1.04875	-0.93286
C	-1.76458	-2.42986	-0.58851
C	-3.10901	-2.97593	-0.61191
C	-3.65550	0.52502	-1.41627
C	0.37716	3.12166	-0.51371
C	3.29678	-0.64639	-1.70019
C	-0.63440	-3.22396	-0.35050
C	0.63231	4.50181	-0.04792
C	4.66592	-0.84014	-2.17531
C	-0.84162	-4.58060	0.19818
C	-5.06019	0.75591	-1.70640
C	0.75245	5.58447	-0.94250
C	0.99588	6.89472	-0.49704
C	1.12624	7.15256	0.87487
C	1.01229	6.09569	1.78838
C	0.76822	4.79107	1.32441
C	-6.10905	0.43278	-0.79196
C	-7.44498	0.64253	-1.07496
C	-7.83583	1.21002	-2.31434
C	-6.81859	1.56949	-3.23740
C	-5.48985	1.35388	-2.93038
C	-1.10153	-5.69268	-0.62865

C	-1.28210	-6.98384	-0.10453
C	-1.20424	-7.19299	1.27950
C	-0.94680	-6.10665	2.12668
C	-0.76926	-4.82153	1.58482
C	5.67130	-1.42257	-1.36885
C	6.98131	-1.62438	-1.83555
C	7.33242	-1.22958	-3.13534
C	6.36359	-0.63170	-3.95578
C	5.05656	-0.44392	-3.47617
H	3.82018	-3.52655	-1.57373
H	1.68147	-4.87527	-0.66923
H	3.09048	3.87880	-0.79174
H	4.66717	1.88409	-1.68219
H	-1.97063	4.74773	-0.62862
H	-4.16825	3.34351	-1.39507
H	-5.00803	-2.00981	-1.19941
Fe	-0.15638	-0.08601	-1.00605
H	-3.36320	-3.98675	-0.38273
F	0.63870	5.37065	-2.24685
F	1.10535	7.89257	-1.37005
F	1.35784	8.38907	1.30521
F	1.13645	6.33329	3.09135
F	0.66632	3.81264	2.21333
F	-5.78085	-0.03945	0.41415
F	-8.38676	0.33265	-0.17739
F	-9.12058	1.40429	-2.60308
F	-7.16831	2.11397	-4.40771
F	-4.56294	1.69071	-3.83065
F	-1.17862	-5.52795	-1.94280
F	-1.52523	-8.01101	-0.91475
F	-1.37265	-8.41202	1.78377
F	-0.87158	-6.29835	3.44117
F	-0.52805	-3.81456	2.41327
F	5.39422	-1.76748	-0.11797
F	7.89735	-2.17880	-1.04587
F	8.57048	-1.41555	-3.58292
F	6.68866	-0.25063	-5.18811
F	4.16491	0.11405	-4.28450