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Dual deoxygenation in α -ketoimine chelated rhenium(III) complex: Structural and mechanistic interpretations

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Dedicated in loving memory of Prof. Amalesh Chandra Banerjee

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1. Computational Methods

DFT calculations in gas phase were carried by employing Gaussian 16 suit of programs.¹ M06-L functional² was used throughout the work along with the 6-31G(d,p)³ basis for the non-metals, and SDD(ECP)⁴ basis for the Re centre. As suggested by one reviewer to check the free energy barriers of OATs with the triple zeta basis set, single point energies at 6-311G(d,p) level were calculated using the optimized geometries obtained from the double zeta calculations. Energy parameters of all the species and a comparative table (Table S1) of energy properties of all the species are provided herewith.

Coordinate details as obtained at M06-L/6-31G(d,p) level of theory

Coordinates of LNOH

O	0.000000	0.000000	0.000000
N	2.334217	-0.328266	-1.575956
C	2.167972	-0.841415	-0.378769
C	1.038994	-0.459233	0.505782
O	1.409889	0.512218	-2.073856
H	0.626193	0.492922	-1.463953
C	3.196796	-1.826287	0.012381
C	2.856343	-2.944500	0.785675
C	4.520542	-1.685671	-0.424948
C	3.817578	-3.890275	1.123323
C	5.478646	-2.633032	-0.085876
C	5.132748	-3.736269	0.692250
H	1.830053	-3.075638	1.120263
H	4.779551	-0.824909	-1.033729
H	3.536085	-4.752722	1.720582
H	6.502548	-2.507096	-0.426363
H	5.884395	-4.473383	0.959499
C	1.147821	-0.520100	1.983552
C	-0.045393	-0.564442	2.718198
C	2.370876	-0.444816	2.665309
C	-0.016602	-0.570032	4.105316
C	2.393808	-0.422378	4.054439
C	1.204048	-0.497965	4.775734
H	-0.984481	-0.594554	2.174161
H	3.301647	-0.384639	2.109767
H	-0.944421	-0.622573	4.667187
H	3.343297	-0.347767	4.575754
H	1.227704	-0.494900	5.861834

Coordinates of OPPh₃

O	0.029716	0.008456	-1.499417
P	0.000000	0.000000	0.000000
C	-0.058572	-1.689763	0.668937
C	-0.048596	-4.331619	1.570368
C	0.208607	-2.735239	-0.219389
C	-0.326545	-1.977565	2.012057
C	-0.320813	-3.293957	2.460622
C	0.213338	-4.052338	0.231724
H	0.399164	-2.494303	-1.262226
H	-0.559364	-1.171420	2.705682
H	-0.533960	-3.512376	3.503263
H	0.418049	-4.861865	-0.463232
H	-0.046190	-5.359723	1.921788
C	1.486085	0.770770	0.709544

C	3.851866	1.901224	1.665732
C	2.518120	1.094769	-0.175117
C	1.645561	1.020200	2.077388
C	2.824515	1.583399	2.553209
C	3.697757	1.658918	0.303480
H	2.371586	0.902519	-1.235019
H	0.839865	0.786542	2.771276
H	2.942452	1.778152	3.615473
H	4.496553	1.911714	-0.388071
H	4.772254	2.341900	2.038824
C	-1.398058	0.857901	0.785329
C	-3.623165	2.217290	1.799867
C	-2.615549	0.190380	0.969568
C	-1.313413	2.217953	1.106635
C	-2.419659	2.892737	1.613175
C	-3.720752	0.866084	1.475669
H	-2.693849	-0.865076	0.718753
H	-0.374674	2.747871	0.962782
H	-2.341923	3.947027	1.863001
H	-4.659100	0.337714	1.618130
H	-4.485998	2.744284	2.197520

Coordinates of HCl

Cl	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.277756

Coordinates of A

Re	9.994082	10.252857	9.938515
Cl	7.716537	10.306652	10.953885
Cl	9.767533	12.668610	9.641632
O	11.465679	10.139692	9.103204
Cl	9.973834	7.881706	10.506733
P	10.795912	10.667524	12.284830
C	10.496905	9.447319	13.608735
C	10.004384	7.721387	15.747965
C	9.323845	8.687144	13.640202
C	11.417070	9.343208	14.660911
C	11.172099	8.480731	15.723170
C	9.084275	7.828456	14.709541
H	8.609747	8.762397	12.826345
H	12.333116	9.929672	14.643676
H	11.894396	8.402331	16.530791
H	8.174002	7.236293	14.723081
H	9.813589	7.046186	16.577594
C	12.593922	10.660249	12.012173
C	15.279299	10.580022	11.257705
C	13.294991	9.448259	12.035666
C	13.239092	11.826939	11.583142

C	14.579461	11.783945	11.215189
C	14.635036	9.414146	11.665268
H	12.786130	8.534163	12.332109
H	12.687125	12.762407	11.528818
H	15.076073	12.693182	10.888975
H	15.174587	8.471836	11.689409
H	16.325306	10.549091	10.966052
C	10.420553	12.264438	13.084353
C	9.794121	14.616775	14.453830
C	11.336408	12.824173	13.985658
C	9.185011	12.887421	12.881093
C	8.878451	14.059443	13.566538
C	11.024122	13.997289	14.663456
H	12.300460	12.347706	14.149413
H	8.472188	12.460432	12.182386
H	7.919495	14.540200	13.397266
H	11.743212	14.426513	15.355427
H	9.551523	15.534269	14.982907
P	8.677856	10.020114	7.779657
C	8.107335	8.344187	7.361462
C	7.448866	5.742596	6.579117
C	9.058612	7.317515	7.440780
C	6.829670	8.058050	6.868350
C	6.503646	6.759653	6.484487
C	8.728685	6.025502	7.050769
H	10.056835	7.534016	7.811070
H	6.092876	8.848649	6.765078
H	5.508650	6.547748	6.103595
H	9.472575	5.237779	7.123146
H	7.190282	4.730564	6.280319
C	7.247312	11.134407	7.658462
C	5.094851	12.917152	7.576053
C	6.042933	10.822118	8.305531
C	7.364709	12.354965	6.983191
C	6.292190	13.239172	6.943457
C	4.972494	11.708054	8.255466
H	5.946759	9.890976	8.854258
H	8.297831	12.617821	6.493400
H	6.396350	14.183599	6.417443
H	4.043692	11.453256	8.757342
H	4.258065	13.609304	7.542274
C	9.734712	10.456912	6.347136
C	11.265389	11.181222	4.120167
C	9.524892	9.834547	5.109365
C	10.716429	11.449644	6.457119
C	11.473652	11.807912	5.345548
C	10.289049	10.195608	4.004333
H	8.766672	9.062396	5.009659
H	10.880054	11.950460	7.407176
H	12.232583	12.578655	5.443655

H	10.120228	9.701700	3.051639
H	11.863548	11.459287	3.256856

Coordinates of B

Re	10.960330	9.945348	9.914978
Cl	11.370611	10.286867	12.318882
O	12.159933	8.722816	9.856510
Cl	10.356852	9.866070	7.533999
P	9.137268	8.240199	10.383973
C	9.182188	7.536376	12.057285
C	9.330550	6.555081	14.667614
C	9.498797	6.193400	12.287835
C	8.960275	8.391675	13.147503
C	9.023478	7.895652	14.444164
C	9.572525	5.707487	13.590479
H	9.684101	5.525821	11.450562
H	8.747505	9.444181	12.974801
H	8.848165	8.564452	15.281588
H	9.817257	4.662871	13.760755
H	9.387653	6.172944	15.683158
C	7.456537	8.928250	10.183051
C	4.916409	10.014276	9.743001
C	7.158362	9.563678	8.969729
C	6.467338	8.831753	11.166128
C	5.204452	9.376844	10.945224
C	5.895629	10.102818	8.754594
H	7.924305	9.634939	8.199746
H	6.678657	8.333332	12.107413
H	4.445695	9.301756	11.718914
H	5.679924	10.600689	7.811902
H	3.932667	10.445931	9.578322
C	9.139139	6.801032	9.262426
C	9.116096	4.545925	7.615275
C	8.014830	5.964192	9.223008
C	10.248517	6.502191	8.466116
C	10.232528	5.375421	7.647125
C	8.005561	4.841274	8.404523
H	7.147117	6.197233	9.837416
H	11.116966	7.152964	8.477035
H	11.095973	5.153022	7.027064
H	7.130397	4.198098	8.380199
H	9.106888	3.670278	6.972039
O	7.598507	13.540362	12.888118
N	8.635352	11.745791	11.047888
C	7.995914	12.816915	10.668589
C	7.124647	13.369109	11.773554
O	9.498267	11.264256	10.144357
C	8.120280	13.545020	9.397453
C	7.897100	14.932457	9.395723

C	8.432231	12.916045	8.179145
C	7.998596	15.672282	8.224808
C	8.519675	13.660726	7.008060
C	8.310977	15.038499	7.024493
H	7.664550	15.437376	10.331133
H	8.603371	11.845981	8.142691
H	7.837081	16.746365	8.251173
H	8.758806	13.151278	6.077006
H	8.387669	15.614806	6.106563
C	5.702948	13.697306	11.483610
C	4.962337	14.331075	12.490606
C	5.074018	13.369980	10.275682
C	3.624569	14.639984	12.291889
C	3.731045	13.673233	10.080936
C	3.006361	14.311732	11.084827
H	5.468741	14.564679	13.422572
H	5.632819	12.866985	9.491678
H	3.058292	15.134823	13.075793
H	3.249333	13.412374	9.142372
H	1.958461	14.552915	10.927912
P	12.510705	11.921237	9.537929
C	11.776744	13.525981	10.014601
C	10.763656	15.976748	10.901979
C	11.137355	13.619093	11.258334
C	11.904947	14.673089	9.220848
C	11.399920	15.891263	9.666780
C	10.631521	14.839357	11.695047
H	11.030956	12.733985	11.881523
H	12.403206	14.619080	8.256927
H	11.501743	16.773763	9.040751
H	10.118221	14.886320	12.651090
H	10.364331	16.928841	11.242702
C	14.065191	11.842236	10.490423
C	16.510533	11.751381	11.834565
C	14.840615	13.001633	10.626959
C	14.520608	10.638837	11.036925
C	15.742405	10.598503	11.704217
C	16.058044	12.954438	11.295912
H	14.485998	13.941674	10.208677
H	13.916817	9.740424	10.956022
H	16.086587	9.661455	12.131913
H	16.651847	13.858221	11.399495
H	17.460313	11.715899	12.361136
C	13.050274	12.125899	7.813176
C	13.768488	12.344574	5.120268
C	14.357595	11.839599	7.406680
C	12.101377	12.506975	6.854146
C	12.462953	12.625672	5.518382
C	14.711567	11.948442	6.064138
H	15.101208	11.536838	8.139279

H	11.079177	12.711956	7.163112
H	11.719086	12.927657	4.785894
H	15.730040	11.726580	5.758295
H	14.049057	12.431162	4.074231

Coordinates of C

Re	10.719684	10.404271	9.883640
Cl	11.012918	11.245322	12.130163
O	11.872351	9.126555	9.821995
Cl	9.812421	10.285147	7.633732
P	9.361071	8.318303	10.625295
C	9.792745	8.080780	12.372084
C	10.709548	8.060374	15.017034
C	11.049352	7.542028	12.684632
C	9.017813	8.636130	13.396786
C	9.469557	8.614111	14.712193
C	11.500111	7.530464	13.999521
H	11.678770	7.144775	11.891454
H	8.059532	9.092810	13.161513
H	8.855034	9.042809	15.498737
H	12.474275	7.107272	14.229114
H	11.063677	8.050271	16.043982
C	7.542676	8.228524	10.503030
C	4.770148	8.079315	10.173581
C	6.923834	8.862562	9.417837
C	6.761464	7.500869	11.408629
C	5.380198	7.433678	11.246204
C	5.544741	8.785536	9.256353
H	7.531878	9.424508	8.711335
H	7.232315	6.991046	12.245978
H	4.781600	6.872313	11.958527
H	5.073319	9.294627	8.419967
H	3.691101	8.032317	10.053213
C	9.924101	6.786902	9.805482
C	10.665509	4.432945	8.493525
C	9.794698	5.547646	10.445908
C	10.423814	6.835812	8.499580
C	10.790792	5.660424	7.849605
C	10.165929	4.377490	9.793145
H	9.410483	5.502109	11.462894
H	10.520812	7.793905	7.994864
H	11.179358	5.707815	6.836259
H	10.064776	3.421669	10.299689
H	10.956474	3.518293	7.984230
O	8.669981	10.978149	10.455029
N	10.207502	12.631491	9.286607
C	8.958541	13.094699	9.540764
C	8.152374	12.102761	10.153794
O	11.024088	13.347850	8.677756

C	8.559968	14.470924	9.212917
C	7.943549	15.271209	10.184272
C	8.781345	15.003250	7.935625
C	7.540805	16.566937	9.882282
C	8.374750	16.298989	7.636941
C	7.753301	17.083672	8.606237
H	7.778068	14.866085	11.179885
H	9.266577	14.391069	7.182247
H	7.064209	17.175158	10.645958
H	8.544717	16.698594	6.641013
H	7.439644	18.096510	8.369077
C	6.713189	12.231893	10.443692
C	6.192323	11.505827	11.524552
C	5.838479	12.946091	9.612372
C	4.830270	11.515539	11.787895
C	4.471707	12.931160	9.865533
C	3.966080	12.225273	10.955420
H	6.879396	10.937662	12.144590
H	6.224916	13.488216	8.754975
H	4.439013	10.954718	12.632033
H	3.798578	13.472186	9.207022
H	2.897585	12.224243	11.152747
P	12.993696	11.593450	9.220601
C	14.340007	10.486398	9.796026
C	16.409472	8.897734	10.818142
C	14.275802	9.989213	11.105404
C	15.457186	10.183493	9.010644
C	16.484795	9.392613	9.519811
C	15.303479	9.200613	11.609719
H	13.411729	10.216724	11.727044
H	15.524433	10.561710	7.993518
H	17.345424	9.163702	8.897058
H	15.235814	8.818405	12.624950
H	17.210430	8.278259	11.212580
C	13.183609	11.607125	7.413486
C	13.270342	11.514501	4.620693
C	13.172064	10.375796	6.743730
C	13.215313	12.790204	6.669940
C	13.263817	12.740938	5.279773
C	13.221440	10.331826	5.355439
H	13.115566	9.452112	7.318005
H	13.192094	13.747599	7.183021
H	13.292717	13.665995	4.710493
H	13.212636	9.372128	4.846362
H	13.306182	11.479645	3.535281
C	13.618716	13.201880	9.828787
C	14.673144	15.593750	10.820698
C	14.849397	13.681763	9.362952
C	12.927254	13.925385	10.804829
C	13.457528	15.113504	11.299357

C	15.368917	14.876258	9.850227
H	15.400360	13.117413	8.612686
H	11.981252	13.549820	11.183268
H	12.913606	15.666576	12.059801
H	16.320400	15.243127	9.475161
H	15.081140	16.524685	11.204954

Coordinates of D

Re	10.158663	10.268126	10.473306
Cl	10.714627	10.956327	12.714234
O	12.168452	9.450615	10.310317
Cl	9.690217	9.477667	8.214543
P	9.283236	8.068923	11.315201
C	8.774028	8.035930	13.064708
C	8.013656	8.116952	15.754574
C	9.738605	8.187580	14.070723
C	7.424657	7.943584	13.420458
C	7.048988	7.986177	14.760585
C	9.359403	8.216511	15.407099
H	10.786112	8.296438	13.801096
H	6.665989	7.842231	12.649074
H	5.997766	7.915559	15.025005
H	10.116199	8.331849	16.177742
H	7.718181	8.147997	16.799710
C	7.852942	7.358781	10.424599
C	5.610868	6.266056	9.170065
C	6.938971	8.192045	9.772833
C	7.636267	5.975051	10.444877
C	6.519197	5.432558	9.819323
C	5.821327	7.641776	9.150722
H	7.098223	9.266792	9.765543
H	8.344335	5.321249	10.949620
H	6.360077	4.357900	9.837194
H	5.117179	8.295358	8.644009
H	4.740058	5.841205	8.677918
C	10.548515	6.753221	11.139608
C	12.417882	4.718923	10.685175
C	10.873986	5.851310	12.158060
C	11.167362	6.623880	9.887060
C	12.091647	5.609992	9.664109
C	11.809636	4.842477	11.930791
H	10.388754	5.925946	13.127331
H	10.919752	7.325684	9.092534
H	12.565499	5.521391	8.690468
H	12.052055	4.146475	12.729712
H	13.146357	3.931510	10.509532
O	10.977528	11.986611	9.708551
N	8.646208	11.546126	10.464088
C	8.859764	12.843500	10.030264

C	10.192709	13.030059	9.650579
O	7.519268	11.148371	10.886733
C	7.750399	13.797290	9.939850
C	7.573158	14.560706	8.776562
C	6.847690	13.962736	11.000072
C	6.537405	15.482237	8.683900
C	5.810108	14.883300	10.900948
C	5.652116	15.647619	9.747164
H	8.258978	14.424318	7.943979
H	6.969893	13.366118	11.897502
H	6.414991	16.065153	7.775124
H	5.120964	15.004827	11.732278
H	4.839047	16.364772	9.674050
C	10.836134	14.279273	9.226377
C	11.935436	14.204392	8.355172
C	10.455150	15.532311	9.729653
C	12.624187	15.353095	7.986402
C	11.152449	16.676805	9.362126
C	12.234969	16.594176	8.487255
H	12.237181	13.230081	7.976410
H	9.624308	15.602197	10.425290
H	13.467574	15.277646	7.304570
H	10.853331	17.639151	9.767953
H	12.774614	17.492819	8.201493
P	13.553778	10.117877	10.289148
C	14.746684	8.804772	10.622229
C	16.561207	6.795484	11.280912
C	14.316390	7.680730	11.336182
C	16.086770	8.915746	10.236130
C	16.990160	7.910982	10.563484
C	15.227709	6.680950	11.664653
H	13.268737	7.592133	11.618394
H	16.420583	9.782263	9.669028
H	18.028359	7.996300	10.256255
H	14.887004	5.808375	12.215108
H	17.268971	6.011798	11.536380
C	13.889587	10.850317	8.677016
C	14.310085	11.964232	6.157654
C	13.060135	10.493688	7.608482
C	14.928581	11.769538	8.480604
C	15.140024	12.319070	7.220241
C	13.271591	11.056188	6.352992
H	12.227316	9.813493	7.773966
H	15.552620	12.075329	9.318111
H	15.942673	13.035847	7.071454
H	12.611650	10.791843	5.532054
H	14.468687	12.405097	5.177246
C	13.849457	11.401942	11.518724
C	14.116939	13.358465	13.486178
C	14.310309	11.056609	12.794976

C	13.532558	12.735765	11.233658
C	13.666241	13.708855	12.215776
C	14.442642	12.034481	13.773359
H	14.556309	10.022014	13.023385
H	13.163518	13.007027	10.249763
H	13.407324	14.738801	11.984351
H	14.796363	11.762378	14.763389
H	14.215800	14.118640	14.256076

Coordinates of E

Re	9.998990	10.543597	10.378192
Cl	10.565109	11.453002	12.606101
O	11.984844	9.867589	10.230607
Cl	10.684205	12.614244	9.335361
P	9.407844	8.307850	11.312705
C	10.868163	7.224936	11.405028
C	13.239405	5.742090	11.428417
C	11.591874	7.023195	10.218237
C	11.354234	6.692306	12.601607
C	12.533284	5.949235	12.608398
C	12.766599	6.281466	10.232131
H	11.237346	7.479752	9.293673
H	10.822673	6.869668	13.533124
H	12.908296	5.547349	13.545870
H	13.323309	6.140722	9.308872
H	14.166286	5.174854	11.441771
C	8.539055	8.189907	12.913686
C	7.046175	7.956527	15.263090
C	8.082526	9.335502	13.571276
C	8.219018	6.923997	13.428220
C	7.485824	6.809513	14.602385
C	7.338320	9.213044	14.743703
H	8.318188	10.317844	13.173337
H	8.541491	6.028800	12.899407
H	7.248308	5.825647	14.997201
H	6.988523	10.108413	15.249150
H	6.467924	7.866534	16.178619
C	8.211874	7.418957	10.238232
C	6.252416	6.206271	8.644422
C	8.507556	6.262297	9.512716
C	6.920726	7.961957	10.157427
C	5.949388	7.359624	9.366094
C	7.529423	5.659719	8.722418
H	9.497224	5.818864	9.571104
H	6.673152	8.854334	10.730463
H	4.954681	7.794688	9.316146
H	7.771473	4.757067	8.168069
H	5.494708	5.737352	8.022860
O	8.075562	11.145689	10.304653

N	9.356789	9.852803	8.594111
C	8.106272	10.268630	8.166557
C	7.435723	10.969191	9.171115
O	10.067110	9.087582	7.873594
C	7.628966	9.961810	6.815492
C	7.135465	10.985328	5.995214
C	7.643500	8.647854	6.328783
C	6.646277	10.698953	4.726188
C	7.151991	8.365843	5.058720
C	6.650311	9.387379	4.254996
H	7.136229	12.007039	6.367134
H	8.032119	7.855012	6.959808
H	6.266085	11.502407	4.101388
H	7.159529	7.341142	4.695824
H	6.267860	9.163430	3.262761
C	6.054282	11.460615	9.147828
C	5.725154	12.562689	9.952206
C	5.039421	10.831781	8.408887
C	4.421620	13.040027	9.993886
C	3.735323	11.308001	8.464211
C	3.422422	12.416331	9.249296
H	6.511927	13.036185	10.531142
H	5.271697	9.959189	7.805536
H	4.183822	13.902455	10.610243
H	2.957721	10.807639	7.893719
H	2.402376	12.788880	9.284097
P	13.467437	10.267792	10.265575
C	14.240231	9.362125	11.626076
C	15.361950	8.066599	13.829111
C	13.548520	9.319934	12.844886
C	15.482833	8.729659	11.512374
C	16.038622	8.082827	12.611830
C	14.117829	8.681786	13.942004
H	12.564805	9.784098	12.925358
H	16.010224	8.725213	10.562209
H	17.001299	7.588755	12.515381
H	13.576892	8.655446	14.884096
H	15.801175	7.565343	14.687413
C	14.208221	9.782894	8.698684
C	15.268994	9.023518	6.238250
C	13.386290	9.171760	7.745446
C	15.554967	10.039360	8.405287
C	16.083918	9.651483	7.179738
C	13.924670	8.794434	6.517147
H	12.326666	9.030838	7.955867
H	16.181787	10.560624	9.126613
H	17.127627	9.849748	6.953981
H	13.282895	8.331563	5.773323
H	15.682880	8.727450	5.278253
C	13.816032	12.016300	10.506284

C	14.165716	14.758279	10.856971
C	13.745986	12.575408	11.787996
C	14.061382	12.841933	9.401211
C	14.243590	14.206771	9.580552
C	13.914775	13.943869	11.957962
H	13.537313	11.948032	12.649238
H	14.083717	12.419794	8.400533
H	14.426811	14.842843	8.719913
H	13.843835	14.373493	12.952429
H	14.296263	15.828207	10.993452

Coordinates of F

Re	8.775417	10.395940	10.170004
Cl	10.402217	9.267154	11.485903
Cl	9.947356	12.460726	10.376148
O	7.663684	10.781794	11.847786
N	7.128126	11.399899	9.533683
C	6.163502	11.768917	10.420395
C	6.510219	11.368252	11.727876
O	7.055839	11.886585	8.252665
C	4.986720	12.537815	9.990370
C	4.685730	13.777433	10.573867
C	4.144935	12.033398	8.984443
C	3.559261	14.484772	10.172965
C	3.022234	12.750827	8.582838
C	2.726111	13.974542	9.178063
H	5.340222	14.171351	11.346688
H	4.370987	11.067048	8.536162
H	3.334413	15.442374	10.632895
H	2.374804	12.348819	7.809176
H	1.848713	14.532666	8.865129
C	5.713551	11.520541	12.944720
C	6.385821	11.506816	14.178030
C	4.312261	11.610506	12.936294
C	5.677250	11.608908	15.367046
C	3.609114	11.705683	14.130331
C	4.287127	11.712998	15.348168
H	7.467450	11.414767	14.178267
H	3.768874	11.567928	11.997306
H	6.211153	11.607636	16.312929
H	2.524503	11.764088	14.110170
H	3.733025	11.792735	16.279213
Cl	9.735879	9.946824	8.049577
H	6.332514	12.541737	8.240687
P	7.614651	8.145820	10.003241
C	6.586098	7.835501	8.525955
C	4.941840	7.329300	6.322622
C	6.477388	8.777113	7.499198
C	5.873542	6.631138	8.433649

C	5.054620	6.381706	7.339462
C	5.654437	8.521067	6.403140
H	7.048610	9.697988	7.539991
H	5.961841	5.888752	9.224500
H	4.507076	5.445595	7.277775
H	5.583549	9.255845	5.606013
H	4.304732	7.131700	5.465044
C	8.649181	6.653516	10.149264
C	10.225210	4.351131	10.230110
C	9.890032	6.628088	9.501152
C	8.205543	5.519718	10.840253
C	8.993877	4.373240	10.879070
C	10.669920	5.477769	9.542378
H	10.245307	7.514035	8.980618
H	7.249562	5.535548	11.358522
H	8.644971	3.498808	11.421114
H	11.634653	5.468519	9.044074
H	10.841371	3.457033	10.265623
C	6.436738	8.047141	11.389674
C	4.727238	8.102582	13.601445
C	5.060340	8.226423	11.213435
C	6.954032	7.924531	12.687613
C	6.100748	7.944470	13.783792
C	4.210768	8.247513	12.318203
H	4.649364	8.340897	10.212618
H	8.029529	7.832082	12.830186
H	6.510651	7.851094	14.785499
H	3.142829	8.386879	12.172461
H	4.064065	8.132274	14.461541

Coordinates of G

Re	8.785320	10.280391	10.817969
Cl	9.448959	8.627829	12.496921
Cl	10.384355	11.556219	12.125949
O	7.225143	10.652438	12.167418
N	8.377907	12.286094	10.575292
C	7.442004	12.789323	11.313481
C	6.733605	11.822819	12.172092
O	7.486358	10.484369	9.277894
C	7.181620	14.245088	11.293812
C	6.961751	14.951757	12.483266
C	7.236913	14.946305	10.084401
C	6.784718	16.330516	12.457881
C	7.048788	16.322905	10.060985
C	6.819898	17.018013	11.246921
H	6.945815	14.419911	13.431325
H	7.435925	14.396886	9.168600
H	6.625691	16.869534	13.387281
H	7.085773	16.856183	9.115477

H	6.677007	18.094600	11.228225
C	5.510233	12.025959	12.941091
C	5.266129	11.177629	14.034748
C	4.539069	12.970506	12.568091
C	4.092538	11.300380	14.762822
C	3.352966	13.063887	13.283636
C	3.133344	12.241094	14.387726
H	6.013087	10.433035	14.293504
H	4.703446	13.608751	11.706133
H	3.918643	10.654243	15.618325
H	2.598116	13.782990	12.980883
H	2.210464	12.330373	14.953869
Cl	10.510307	9.851221	9.260057
H	7.632863	11.356734	8.883374
P	7.661226	7.998742	10.190045
C	7.005359	7.859570	8.492331
C	6.171830	7.449488	5.857039
C	7.808829	8.279895	7.425065
C	5.787851	7.223278	8.228509
C	5.373351	7.023578	6.913903
C	7.390764	8.073714	6.115916
H	8.752670	8.779078	7.630686
H	5.160254	6.881629	9.047745
H	4.424849	6.530789	6.719358
H	8.018617	8.406784	5.294485
H	5.846696	7.292830	4.832247
C	8.576204	6.430977	10.349187
C	9.929080	3.990181	10.353515
C	9.969317	6.401710	10.231776
C	7.863714	5.229843	10.452563
C	8.541143	4.014765	10.462690
C	10.638497	5.182340	10.232648
H	10.524444	7.332254	10.152810
H	6.778315	5.244980	10.527322
H	7.981827	3.087894	10.552628
H	11.720873	5.167828	10.146457
H	10.457332	3.040851	10.360802
C	6.220781	7.902455	11.285994
C	4.071568	8.010915	13.065610
C	5.103743	8.700548	10.997877
C	6.266192	7.187207	12.487068
C	5.188316	7.236454	13.367277
C	4.033799	8.749002	11.883349
H	5.089029	9.290245	10.083480
H	7.147176	6.600412	12.732116
H	5.226489	6.670021	14.293386
H	3.172842	9.372799	11.656171
H	3.233207	8.050417	13.756224

Coordinates of H

Re	9.486571	11.471769	9.850515
Cl	11.121208	9.699800	9.813635
Cl	11.062895	13.114717	10.426484
O	9.347299	10.869262	11.897170
N	8.018961	12.258919	10.497589
C	7.473962	12.173445	11.730187
C	8.276089	11.276007	12.495211
O	8.145172	9.746554	8.812779
C	6.365210	13.051338	12.101582
C	6.101165	13.446894	13.424918
C	5.557378	13.590416	11.083179
C	5.046826	14.303356	13.715076
C	4.508516	14.453087	11.378169
C	4.235972	14.805841	12.698247
H	6.742577	13.097962	14.228230
H	5.782837	13.330638	10.051400
H	4.869008	14.596595	14.746357
H	3.905188	14.858226	10.568876
H	3.416465	15.479615	12.930880
C	7.993365	10.702566	13.814721
C	9.062410	10.263059	14.611695
C	6.682315	10.480610	14.261046
C	8.823120	9.639887	15.829857
C	6.446742	9.854790	15.479199
C	7.515432	9.435305	16.270466
H	10.074173	10.418050	14.249303
H	5.846405	10.787847	13.636743
H	9.660137	9.314673	16.441807
H	5.424768	9.684839	15.808367
H	7.330089	8.951123	17.225494
Cl	9.447058	11.854453	7.456172
H	8.251653	10.192154	7.922412
P	6.893166	8.773973	9.078275
C	7.111068	7.408142	7.940704
C	7.541429	5.193726	6.315689
C	8.369435	7.207889	7.356432
C	6.077630	6.483633	7.730698
C	6.296158	5.381473	6.913978
C	8.573914	6.100762	6.539335
H	9.182355	7.904642	7.547952
H	5.107678	6.627273	8.202576
H	5.495577	4.668064	6.745466
H	9.545708	5.948384	6.081034
H	7.708264	4.331327	5.677337
C	7.068166	8.263644	10.770038
C	7.369362	7.231145	13.327921
C	8.355361	8.090104	11.298017
C	5.931952	7.901339	11.512429

C	6.091351	7.386766	12.791941
C	8.492677	7.585611	12.586331
H	9.238095	8.382945	10.731239
H	4.935502	8.035744	11.097933
H	5.216941	7.123864	13.379575
H	9.486805	7.491989	13.012237
H	7.486885	6.854295	14.339817
C	5.332813	9.595908	8.816089
C	2.982727	11.028124	8.412043
C	4.605797	9.427315	7.627558
C	4.891442	10.507857	9.789653
C	3.713171	11.214775	9.584257
C	3.430630	10.142817	7.433501
H	4.959158	8.743669	6.860613
H	5.477402	10.677331	10.693187
H	3.384281	11.925748	10.336294
H	2.867155	10.012090	6.515120
H	2.063914	11.585288	8.254695

Coordinates of I

Re	10.309043	11.934445	10.163711
Cl	8.694416	10.873981	8.688500
Cl	12.087250	12.655543	11.565617
O	9.508824	10.848241	11.699313
N	8.938362	13.118092	10.936771
C	8.137978	12.671084	11.921086
C	8.477849	11.357927	12.319268
O	8.846889	15.818755	10.374002
C	7.095921	13.551071	12.472618
C	6.991912	13.796449	13.848086
C	6.213721	14.199107	11.597740
C	6.030227	14.675891	14.332717
C	5.251820	15.076564	12.085924
C	5.159797	15.320650	13.454597
H	7.677790	13.301842	14.531280
H	6.283862	13.997227	10.531716
H	5.966259	14.866463	15.400392
H	4.577323	15.572511	11.391880
H	4.411950	16.010196	13.837153
C	7.837463	10.529347	13.337679
C	8.612070	9.565798	14.002962
C	6.469034	10.624723	13.639398
C	8.040209	8.739075	14.960167
C	5.901519	9.788340	14.592324
C	6.683468	8.847539	15.261068
H	9.665136	9.484571	13.751783
H	5.847506	11.339609	13.109155
H	8.656023	8.004337	15.473403
H	4.839784	9.866100	14.808671

H	6.235571	8.199585	16.009447
Cl	10.993160	13.361593	8.394451
H	8.848358	14.122578	10.680652
P	8.191224	16.491669	9.191192
C	7.339540	18.001778	9.717851
C	5.908352	20.203804	10.656942
C	6.962869	18.072916	11.063590
C	7.007247	19.045442	8.848417
C	6.293978	20.143791	9.318765
C	6.244616	19.170441	11.528430
H	7.245848	17.263181	11.732256
H	7.314773	19.003206	7.805232
H	6.041543	20.955514	8.642292
H	5.951963	19.219554	12.573923
H	5.350537	21.062252	11.021148
C	9.376339	16.921391	7.898630
C	11.284021	17.556498	5.971612
C	10.732417	16.940198	8.237532
C	8.980597	17.203164	6.585881
C	9.933880	17.527748	5.626555
C	11.682573	17.256835	7.271930
H	11.028145	16.670406	9.247828
H	7.928432	17.143999	6.310713
H	9.626214	17.742884	4.607091
H	12.736762	17.254855	7.532761
H	12.028973	17.799024	5.218635
C	6.931337	15.462600	8.390194
C	5.036452	13.687468	7.363702
C	5.587578	15.842636	8.298434
C	7.320774	14.184737	7.960138
C	6.373390	13.302136	7.452483
C	4.644714	14.956479	7.782567
H	5.275688	16.826421	8.642548
H	8.361917	13.868221	8.035511
H	6.688878	12.309485	7.145679
H	3.602375	15.256370	7.715411
H	4.297210	12.994327	6.971213
O	11.694907	10.422843	9.556917
P	11.674679	8.919991	9.255096
C	11.198348	8.617787	7.548425
C	10.546582	8.238876	4.871167
C	11.207499	9.706617	6.669135
C	10.850782	7.342767	7.087349
C	10.527979	7.155593	5.747390
C	10.881217	9.510258	5.331789
H	11.437505	10.701193	7.046060
H	10.808623	6.503067	7.778929
H	10.252666	6.167666	5.389901
H	10.876652	10.356745	4.651941
H	10.288447	8.091829	3.826060

C	13.364285	8.348148	9.524498
C	15.970586	7.514647	10.030231
C	14.268031	9.223276	10.136599
C	13.767937	7.057254	9.165780
C	15.070170	6.643130	9.418465
C	15.570607	8.799344	10.387396
H	13.939244	10.223677	10.407597
H	13.066334	6.377808	8.685409
H	15.384279	5.642203	9.137287
H	16.273151	9.477587	10.862421
H	16.988325	7.189059	10.226660
C	10.609735	7.943849	10.330961
C	8.920057	6.649002	12.129923
C	9.257973	7.757007	10.014570
C	11.109975	7.474547	11.553137
C	10.265610	6.825201	12.446040
C	8.418616	7.112396	10.916283
H	8.865199	8.138871	9.076791
H	12.158503	7.620648	11.802658
H	10.655783	6.464768	13.394048
H	7.368485	6.981016	10.673517
H	8.257846	6.156764	12.837030

Coordinates of 1

Re	9.978304	10.233094	10.519710
Cl	10.601487	10.796820	12.756292
O	11.962752	9.486735	10.226204
Cl	9.538379	9.589807	8.249513
O	10.645464	12.063346	9.925193
N	8.372460	11.402642	10.619576
C	8.497442	12.726262	10.379769
C	9.822594	13.074645	10.030761
C	7.320533	13.599787	10.425348
C	7.092195	14.561900	9.429869
C	6.370677	13.442428	11.445229
C	5.949592	15.350142	9.462986
C	5.226873	14.232847	11.473058
C	5.013622	15.189321	10.483786
H	7.812470	14.675915	8.624306
H	6.551133	12.714561	12.233363
H	5.781857	16.085497	8.681396
H	4.504717	14.105522	12.274202
H	4.119956	15.806088	10.505847
C	10.399205	14.396588	9.797968
C	11.525996	14.495228	8.962336
C	9.936410	15.550269	10.450706
C	12.159892	15.715879	8.774866
C	10.578451	16.767633	10.260903
C	11.688380	16.857459	9.421830

H	11.890287	13.598259	8.466010
H	9.089886	15.484120	11.127452
H	13.025169	15.775314	8.119763
H	10.217246	17.649956	10.781376
H	12.186166	17.812167	9.277771
P	13.342549	10.174900	10.218032
C	14.558095	8.845889	10.232817
C	16.409718	6.768951	10.188333
C	14.119644	7.525455	10.095890
C	15.925462	9.124345	10.346693
C	16.848153	8.085560	10.324787
C	15.050464	6.490342	10.075580
H	13.055155	7.325426	10.015853
H	16.266020	10.151679	10.463947
H	17.908456	8.301331	10.417181
H	14.710453	5.464141	9.974024
H	17.132490	5.958141	10.172633
C	13.567133	11.159753	8.721165
C	13.864115	12.638465	6.376899
C	12.719126	10.924431	7.634344
C	14.573312	12.130104	8.625648
C	14.720315	12.864857	7.453919
C	12.867175	11.669959	6.468195
H	11.923854	10.187486	7.717792
H	15.224966	12.328580	9.473930
H	15.496978	13.621381	7.385733
H	12.193479	11.494992	5.634647
H	13.974545	13.221011	5.466358
C	13.705656	11.264298	11.602789
C	14.047019	12.912084	13.823679
C	14.242203	10.743848	12.786517
C	13.338257	12.614871	11.541296
C	13.511589	13.434610	12.648471
C	14.413356	11.569565	13.891436
H	14.515124	9.693061	12.844774
H	12.899109	13.017189	10.632947
H	13.217310	14.479415	12.591630
H	14.825875	11.162546	14.809618
H	14.176437	13.551795	14.692174
Cl	9.011977	8.229391	11.275464
H	7.427152	11.067879	10.785855

Coordinates of TS1

Re	10.024302	11.039042	9.334244
Cl	10.195844	11.601057	11.732038
O	11.334774	9.613330	9.095030
Cl	9.281600	10.682159	7.087264
P	9.926781	8.669155	9.927503
C	11.105264	7.985274	11.149151

C	12.921654	6.837983	12.953527
C	11.928918	6.921831	10.755220
C	11.222218	8.481821	12.453788
C	12.126132	7.910704	13.345110
C	12.823586	6.348936	11.654063
H	11.867209	6.536416	9.741033
H	10.617010	9.325100	12.768517
H	12.209841	8.315272	14.350345
H	13.447247	5.518657	11.333041
H	13.622374	6.392038	13.654821
C	8.265210	8.305842	10.714127
C	5.657850	7.893621	11.677349
C	7.150257	8.484130	9.879087
C	8.046557	7.938518	12.045117
C	6.750527	7.734777	12.522910
C	5.861694	8.270037	10.349002
H	7.304224	8.796831	8.846245
H	8.886756	7.777562	12.713893
H	6.601503	7.436604	13.557632
H	5.013173	8.409070	9.684251
H	4.649671	7.728668	12.049132
C	9.837164	7.459493	8.548992
C	9.804831	5.471837	6.567309
C	9.150118	6.253359	8.752943
C	10.522326	7.646076	7.342014
C	10.493754	6.662997	6.357402
C	9.140070	5.266222	7.772737
H	8.628816	6.076454	9.689374
H	11.070042	8.566858	7.179207
H	11.017127	6.833067	5.420635
H	8.607902	4.336567	7.954207
H	9.789416	4.705333	5.797058
O	8.014372	11.219164	9.861175
N	9.422930	13.062950	8.897751
C	8.251721	13.495044	9.449054
C	7.503428	12.398846	9.943869
O	10.139449	13.811380	8.197112
C	7.947075	14.924887	9.565725
C	7.571586	15.433198	10.820148
C	8.103241	15.812676	8.493076
C	7.341946	16.792019	10.992307
C	7.873806	17.173439	8.673116
C	7.492881	17.667394	9.917643
H	7.473931	14.749937	11.661231
H	8.406385	15.431109	7.525372
H	7.054426	17.169720	11.969581
H	7.995940	17.851695	7.833292
H	7.317685	18.731149	10.052368
C	6.161627	12.463615	10.530631
C	5.820113	11.495144	11.487446

C	5.207320	13.415211	10.140040
C	4.555466	11.497353	12.060345
C	3.939163	13.399228	10.705532
C	3.613325	12.448027	11.671725
H	6.563735	10.755400	11.771774
H	5.454159	14.150234	9.380253
H	4.305029	10.751028	12.809155
H	3.200468	14.129477	10.388737
H	2.622199	12.445549	12.117008
P	12.370032	12.134292	9.436071
C	12.536180	13.910127	9.853328
C	12.832010	16.619698	10.487937
C	11.572968	14.565820	10.630116
C	13.650198	14.626616	9.401121
C	13.797571	15.972852	9.721903
C	11.720542	15.913276	10.940307
H	10.703435	14.021478	10.987671
H	14.400827	14.135119	8.787253
H	14.666069	16.517628	9.362295
H	10.953008	16.412133	11.526001
H	12.942813	17.673848	10.726788
C	13.401271	11.282823	10.667723
C	14.909125	9.946746	12.607181
C	13.629901	11.871433	11.917152
C	13.924860	10.008367	10.404152
C	14.681024	9.352480	11.368620
C	14.379138	11.204308	12.880883
H	13.214908	12.851362	12.136997
H	13.733493	9.534044	9.447113
H	15.077186	8.363628	11.155734
H	14.548747	11.672042	13.846620
H	15.493461	9.424848	13.360929
C	13.238594	11.938624	7.845741
C	14.517632	11.718107	5.368748
C	14.614331	11.679852	7.779400
C	12.512296	12.095984	6.659338
C	13.151828	11.982996	5.429003
C	15.248236	11.571945	6.545049
H	15.190300	11.562842	8.693613
H	11.448149	12.308797	6.704273
H	12.575914	12.099254	4.515488
H	16.315219	11.371003	6.505160
H	15.013245	11.626351	4.406130

Coordinates of TS2

Re	8.633195	10.426562	10.036735
Cl	10.111835	9.263686	11.429522
Cl	9.879698	12.465986	10.289252
O	7.797405	10.916662	11.851838

N	6.666242	10.847560	9.621692
C	5.978916	11.560927	10.604518
C	6.586869	11.436132	11.847487
O	7.518977	11.740654	8.652810
C	4.745582	12.234535	10.194347
C	4.325814	13.425772	10.808875
C	3.990762	11.731582	9.121464
C	3.168796	14.068871	10.389530
C	2.838130	12.384044	8.701084
C	2.417338	13.550914	9.335644
H	4.917009	13.843148	11.619993
H	4.324802	10.823385	8.625293
H	2.860279	14.988784	10.878241
H	2.263925	11.977912	7.872810
H	1.516733	14.059672	9.004461
C	6.022783	11.710738	13.174380
C	6.904414	11.921360	14.244777
C	4.643171	11.677838	13.424064
C	6.414135	12.118296	15.530105
C	4.159775	11.865199	14.712054
C	5.041820	12.091095	15.768313
H	7.971823	11.921707	14.048151
H	3.952849	11.472010	12.611677
H	7.106412	12.288453	16.349616
H	3.089455	11.824892	14.894825
H	4.659597	12.239485	16.774428
Cl	9.793280	9.812282	8.052730
H	7.614942	12.622988	9.074587
P	7.485982	8.158201	9.852025
C	6.662340	7.828849	8.259924
C	5.331944	7.244258	5.874481
C	6.576405	8.792840	7.250128
C	6.085125	6.566648	8.060793
C	5.419727	6.278488	6.875016
C	5.911810	8.495280	6.062945
H	7.031251	9.768458	7.380959
H	6.160385	5.808250	8.837669
H	4.975524	5.297893	6.730883
H	5.855491	9.247056	5.281312
H	4.816744	7.017901	4.945191
C	8.476896	6.666548	10.169259
C	9.993957	4.348719	10.514286
C	9.728451	6.545994	9.551354
C	7.992380	5.619345	10.961289
C	8.751975	4.464649	11.131025
C	10.479056	5.389538	9.725019
H	10.114892	7.365742	8.950657
H	7.024050	5.705679	11.447597
H	8.370064	3.656984	11.748833
H	11.451473	5.306749	9.248921

H	10.586609	3.448700	10.651711
C	6.166709	8.152193	11.100771
C	4.212125	8.329069	13.085333
C	4.814908	8.227802	10.750913
C	6.536006	8.186027	12.454467
C	5.559535	8.268521	13.439336
C	3.841954	8.314676	11.743911
H	4.523875	8.221354	9.703511
H	7.590265	8.172863	12.726266
H	5.851560	8.311812	14.485071
H	2.794058	8.377285	11.464107
H	3.453036	8.408800	13.858760

Coordinates of TS3

Re	9.162263	11.222919	9.694899
Cl	10.576515	9.305620	9.389709
Cl	10.883776	12.310617	10.885235
O	8.938586	10.288464	11.624357
N	7.810694	12.085733	10.532348
C	7.374531	11.944452	11.788924
C	8.088811	10.869316	12.396965
O	7.918920	10.289997	8.049378
C	6.421813	12.901578	12.369472
C	6.666905	13.516787	13.606173
C	5.267031	13.260493	11.661514
C	5.771278	14.443977	14.124065
C	4.375709	14.194812	12.178176
C	4.621328	14.786665	13.414316
H	7.573168	13.268521	14.152201
H	5.073196	12.789341	10.700165
H	5.980710	14.914519	15.080684
H	3.484583	14.458806	11.614705
H	3.925753	15.516043	13.819276
C	7.988023	10.378010	13.775099
C	9.088940	9.693709	14.314197
C	6.825604	10.511073	14.548621
C	9.030954	9.170135	15.599226
C	6.771672	9.982093	15.832362
C	7.873622	9.313598	16.363443
H	9.980466	9.589464	13.703133
H	5.953556	11.005186	14.131566
H	9.893232	8.651398	16.008634
H	5.862792	10.086657	16.418664
H	7.829885	8.905629	17.369605
Cl	9.482269	12.527355	7.765561
H	7.466862	10.987577	7.536905
P	7.027233	9.151546	8.946827
C	7.576236	7.672460	8.081394
C	8.325805	5.356741	6.711297

C	8.513520	7.742056	7.041175
C	7.025354	6.428897	8.433556
C	7.392079	5.280681	7.742410
C	8.886908	6.583681	6.368655
H	8.970569	8.691246	6.788442
H	6.315377	6.359761	9.253792
H	6.956259	4.325195	8.018113
H	9.628971	6.643127	5.578633
H	8.621805	4.456614	6.180357
C	6.727004	8.587837	10.633791
C	6.249798	7.530118	13.166873
C	7.683693	7.753617	11.240221
C	5.572558	8.959019	11.342774
C	5.331294	8.408662	12.596463
C	7.431204	7.216909	12.493883
H	8.618192	7.545843	10.723259
H	4.850735	9.642062	10.902299
H	4.426346	8.676898	13.134257
H	8.167842	6.567847	12.957671
H	6.063355	7.118813	14.154822
C	5.387706	9.716020	8.402157
C	2.843519	10.604250	7.677766
C	4.407435	8.797439	8.016042
C	5.085359	11.084667	8.427424
C	3.813356	11.523164	8.070360
C	3.142248	9.243848	7.647705
H	4.638920	7.734828	7.991213
H	5.833876	11.806994	8.754999
H	3.584620	12.584570	8.100416
H	2.388792	8.527095	7.335311
H	1.853523	10.948407	7.393795

Coordinates of C'

Re	-0.024640000	0.184989000	-0.281768000
Cl	-0.004606000	1.412602000	1.820159000
O	0.219347000	-1.402661000	0.373243000
Cl	-0.016704000	-0.471415000	-2.665965000
P	-2.381669000	-0.780897000	0.064870000
C	-2.719594000	-0.590898000	1.835897000
C	-2.875186000	-0.130589000	4.591277000
C	-2.219558000	-1.536260000	2.741844000
C	-3.265812000	0.601512000	2.326966000
C	-3.354437000	0.822415000	3.696552000
C	-2.301603000	-1.305531000	4.110974000
H	-1.758564000	-2.448833000	2.371485000
H	-3.607947000	1.365403000	1.632413000
H	-3.784792000	1.749499000	4.064200000
H	-1.916794000	-2.048340000	4.804598000
H	-2.939473000	0.046399000	5.661274000

C	-3.821153000	-0.101294000	-0.820479000
C	-5.983019000	0.871679000	-2.298578000
C	-3.639285000	0.315156000	-2.145664000
C	-5.096432000	-0.039469000	-0.247742000
C	-6.171392000	0.451572000	-0.984632000
C	-4.718189000	0.795919000	-2.878882000
H	-2.645240000	0.275461000	-2.585797000
H	-5.247640000	-0.365195000	0.778876000
H	-7.156966000	0.503250000	-0.530097000
H	-4.568032000	1.121467000	-3.904269000
H	-6.822406000	1.257118000	-2.870924000
C	-2.500352000	-2.581245000	-0.229113000
C	-2.777566000	-5.315476000	-0.748245000
C	-3.535509000	-3.316130000	0.364740000
C	-1.609374000	-3.228760000	-1.091624000
C	-1.751470000	-4.590511000	-1.346614000
C	-3.671811000	-4.675584000	0.107867000
H	-4.231328000	-2.820301000	1.038827000
H	-0.808897000	-2.667974000	-1.565760000
H	-1.053524000	-5.083827000	-2.017676000
H	-4.476435000	-5.235523000	0.576333000
H	-2.883397000	-6.378233000	-0.948534000
O	-1.488585000	1.664767000	-0.706248000
N	1.013865000	1.946131000	-1.212123000
O	2.107290000	1.668794000	-2.036113000
P	2.627660000	-0.201668000	0.052116000
C	2.906243000	-1.312725000	1.483839000
C	3.432243000	-2.939600000	3.701434000
C	2.053414000	-1.293498000	2.593099000
C	4.028123000	-2.152568000	1.501745000
C	4.289488000	-2.959722000	2.603659000
C	2.317998000	-2.105773000	3.692408000
H	1.182970000	-0.644067000	2.597393000
H	4.695374000	-2.183570000	0.642997000
H	5.162358000	-3.606753000	2.602334000
H	1.643751000	-2.083739000	4.544419000
H	3.633964000	-3.573191000	4.560934000
C	3.180884000	-1.218418000	-1.352955000
C	3.659905000	-2.785869000	-3.626153000
C	2.698868000	-2.534564000	-1.426907000
C	3.894658000	-0.696245000	-2.438896000
C	4.137396000	-1.480122000	-3.564111000
C	2.938872000	-3.309316000	-2.554940000
H	2.121906000	-2.941694000	-0.599628000
H	4.256706000	0.328143000	-2.404438000
H	4.698955000	-1.064040000	-4.395947000
H	2.555221000	-4.325043000	-2.599272000
H	3.845064000	-3.392464000	-4.508090000
C	3.868977000	1.109364000	0.313106000
C	5.701131000	3.149037000	0.863844000

C	5.225974000	0.941568000	0.012343000
C	3.441591000	2.300041000	0.914044000
C	4.356433000	3.313611000	1.185247000
C	6.134907000	1.959758000	0.282408000
H	5.572494000	0.012779000	-0.435353000
H	2.392777000	2.417569000	1.182076000
H	4.015467000	4.233013000	1.653492000
H	7.185410000	1.821439000	0.041610000
H	6.413319000	3.942352000	1.073616000
C	-2.766290000	3.555028000	-0.154166000
C	-1.526196000	2.940552000	-0.438864000
C	-0.364852000	3.767479000	-0.495934000
C	-0.464646000	5.142860000	-0.209163000
C	-1.676256000	5.705928000	0.133826000
C	-2.829357000	4.901855000	0.145016000
H	-3.656462000	2.930400000	-0.166271000
H	0.433002000	5.754944000	-0.268423000
H	-1.744468000	6.762864000	0.369695000
H	-3.790062000	5.347460000	0.390677000
C	0.814226000	3.224997000	-1.072699000
H	1.559245000	3.886628000	-1.516635000
H	1.791420000	0.879653000	-2.530449000

Coordinates of H'

Re	0.716057000	-1.402127000	0.055734000
Cl	0.938701000	-1.291173000	2.510416000
O	-0.434060000	-2.699440000	0.095966000
Cl	0.758129000	-1.313011000	-2.443099000
P	-1.271316000	0.209695000	0.014905000
C	-2.067290000	0.473520000	1.635891000
C	-3.118048000	0.831378000	4.204492000
C	-3.361425000	0.040383000	1.936962000
C	-1.292486000	1.065880000	2.644436000
C	-1.821708000	1.253553000	3.915416000
C	-3.883284000	0.219333000	3.216424000
H	-3.964348000	-0.438232000	1.169700000
H	-0.270342000	1.365586000	2.425432000
H	-1.210572000	1.712449000	4.687849000
H	-4.891583000	-0.121519000	3.438346000
H	-3.526589000	0.970286000	5.202589000
C	-0.908026000	1.909045000	-0.570065000
C	-0.354639000	4.450338000	-1.604562000
C	-0.130714000	2.047242000	-1.728271000
C	-1.406465000	3.053160000	0.059291000
C	-1.127060000	4.318728000	-0.455327000
C	0.137951000	3.311109000	-2.240093000
H	0.275785000	1.157206000	-2.206531000
H	-2.009562000	2.959689000	0.959081000
H	-1.515614000	5.200983000	0.047867000
H	0.752868000	3.405377000	-3.131291000
H	-0.132700000	5.437806000	-2.002580000
C	-2.660821000	-0.264218000	-1.085493000

C	-4.794893000	-0.951323000	-2.758099000
C	-3.711913000	0.637219000	-1.305790000
C	-2.683439000	-1.509601000	-1.719594000
C	-3.750397000	-1.846517000	-2.551145000
C	-4.775082000	0.294850000	-2.133093000
H	-3.691297000	1.613623000	-0.824013000
H	-1.864831000	-2.204757000	-1.561512000
H	-3.756505000	-2.815196000	-3.043683000
H	-5.584990000	1.002088000	-2.294633000
H	-5.622947000	-1.219280000	-3.410307000
O	1.583047000	0.505139000	0.045525000
N	2.491999000	-2.038523000	-0.003316000
C	3.164099000	2.234094000	-0.002989000
C	2.847678000	0.857240000	-0.004204000
C	3.917684000	-0.083008000	-0.060463000
C	5.238312000	0.390601000	-0.114950000
C	5.530000000	1.744385000	-0.116444000
C	4.477319000	2.667917000	-0.058737000
H	2.334158000	2.935980000	0.043423000
H	6.041234000	-0.346013000	-0.155162000
H	6.561195000	2.085935000	-0.159764000
H	4.690927000	3.735209000	-0.057108000
C	3.656220000	-1.506317000	-0.052809000
H	4.539758000	-2.161881000	-0.089158000

Coordinates of I'

Re	1.373738000	0.112228000	-1.547241000
Cl	3.387873000	0.076105000	-2.854351000
O	0.711717000	-1.431738000	-1.875286000
Cl	0.272829000	1.423352000	-3.265441000
P	2.586303000	-0.939540000	0.375861000
C	3.848665000	-2.173335000	-0.082544000
C	5.677819000	-4.171407000	-0.755506000
C	4.953278000	-2.424234000	0.740240000
C	3.666054000	-2.931012000	-1.244434000
C	4.578866000	-3.927709000	-1.574702000
C	5.864911000	-3.418542000	0.401397000
H	5.107738000	-1.831658000	1.639381000
H	2.818907000	-2.729701000	-1.894397000
H	4.435163000	-4.505466000	-2.482840000
H	6.723317000	-3.603206000	1.041151000
H	6.392916000	-4.945116000	-1.020773000
C	3.469498000	0.316836000	1.344019000
C	4.776945000	2.415814000	2.644898000
C	2.923752000	0.878401000	2.503548000
C	4.659801000	0.839297000	0.820299000
C	5.311328000	1.878380000	1.474857000
C	3.580418000	1.920234000	3.153221000
H	1.982874000	0.503891000	2.899450000
H	5.061847000	0.437917000	-0.107883000
H	6.235498000	2.274674000	1.064010000
H	3.146035000	2.351869000	4.050624000
H	5.286425000	3.231211000	3.151044000
C	1.527887000	-1.838225000	1.568517000

C	-0.070466000	-3.269919000	3.366796000
C	2.009328000	-2.163494000	2.845331000
C	0.247100000	-2.260573000	1.195612000
C	-0.545868000	-2.972649000	2.093540000
C	1.212506000	-2.869678000	3.739247000
H	3.008682000	-1.852340000	3.142518000
H	-0.140779000	-2.049843000	0.204861000
H	-1.542202000	-3.279089000	1.786775000
H	1.594717000	-3.109488000	4.727622000
H	-0.693925000	-3.818637000	4.067869000
O	2.034453000	1.855582000	-0.748869000
N	-0.257174000	0.564122000	-0.294360000
P	-3.806658000	-0.509535000	-0.046210000
C	-5.191768000	-1.280794000	-0.912831000
C	-7.288070000	-2.559521000	-2.230063000
C	-5.055539000	-2.612296000	-1.317976000
C	-6.377453000	-0.588054000	-1.182986000
C	-7.424914000	-1.229989000	-1.835883000
C	-6.103816000	-3.247776000	-1.975999000
H	-4.117707000	-3.128307000	-1.129583000
H	-6.470896000	0.459320000	-0.899844000
H	-8.342675000	-0.689597000	-2.049041000
H	-5.994039000	-4.279347000	-2.297574000
H	-8.103810000	-3.056880000	-2.747111000
C	-4.204839000	-0.527430000	1.724236000
C	-4.640529000	-0.542414000	4.481555000
C	-5.506043000	-0.446004000	2.230654000
C	-3.124494000	-0.624052000	2.608991000
C	-3.342957000	-0.634599000	3.982753000
C	-5.720689000	-0.448844000	3.606087000
H	-6.352849000	-0.395576000	1.548582000
H	-2.116718000	-0.718171000	2.208585000
H	-2.498738000	-0.722977000	4.661362000
H	-6.733058000	-0.388460000	3.995173000
H	-4.812602000	-0.552019000	5.554201000
C	-3.763013000	1.231450000	-0.537643000
C	-3.436515000	3.898834000	-1.285604000
C	-4.365616000	2.250134000	0.211584000
C	-2.998445000	1.559374000	-1.665557000
C	-2.832104000	2.890398000	-2.033095000
C	-4.206276000	3.579745000	-0.168094000
H	-4.939316000	2.004848000	1.103396000
H	-2.488760000	0.781693000	-2.231236000
H	-2.202601000	3.127464000	-2.885367000
H	-4.670195000	4.368052000	0.418268000
H	-3.297175000	4.938819000	-1.567151000
C	2.447303000	3.872083000	0.382930000
C	1.629924000	2.762443000	0.110837000
C	0.375831000	2.653548000	0.769591000
C	-0.009451000	3.645462000	1.686296000
C	0.813168000	4.724839000	1.959812000
C	2.042159000	4.831780000	1.296382000
H	3.398698000	3.940801000	-0.134360000
H	-0.977117000	3.547648000	2.176582000
H	0.505332000	5.484313000	2.671405000

H	2.691924000	5.679237000	1.500104000
C	-0.503303000	1.552482000	0.504574000
H	-1.470251000	1.561009000	1.020571000
O	-2.492461000	-1.209126000	-0.313200000
H	-1.037325000	-0.109163000	-0.361548000

Energy details as obtained at M06-L/6-31G(d,p) level of theory

LNOH

Zero-point correction=	0.217896 (Hartree/Particle)
Thermal correction to Energy=	0.231361
Thermal correction to Enthalpy=	0.232306
Thermal correction to Gibbs Free Energy=	0.176642
Sum of electronic and zero-point Energies=	-744.967392
Sum of electronic and thermal Energies=	-744.953926
Sum of electronic and thermal Enthalpies=	-744.952982
Sum of electronic and thermal Free Energies=	-745.008645

OPPh₃

Zero-point correction=	0.278374 (Hartree/Particle)
Thermal correction to Energy=	0.295175
Thermal correction to Enthalpy=	0.296119
Thermal correction to Gibbs Free Energy=	0.231260
Sum of electronic and zero-point Energies=	-1111.183052
Sum of electronic and thermal Energies=	-1111.166252
Sum of electronic and thermal Enthalpies=	-1111.165308
Sum of electronic and thermal Free Energies=	-1111.230167

HCl

Zero-point correction=	0.006917 (Hartree/Particle)
Thermal correction to Energy=	0.009278
Thermal correction to Enthalpy=	0.010222
Thermal correction to Gibbs Free Energy=	-0.010958
Sum of electronic and zero-point Energies=	-460.771665
Sum of electronic and thermal Energies=	-460.769305
Sum of electronic and thermal Enthalpies=	-460.768361
Sum of electronic and thermal Free Energies=	-460.789541

A

Zero-point correction=	0.558875 (Hartree/Particle)
Thermal correction to Energy=	0.600645
Thermal correction to Enthalpy=	0.601589
Thermal correction to Gibbs Free Energy=	0.479497
Sum of electronic and zero-point Energies=	-3606.160207
Sum of electronic and thermal Energies=	-3606.118436

Sum of electronic and thermal Enthalpies=	-3606.117492
Sum of electronic and thermal Free Energies=	-3606.239584

B

Zero-point correction=	0.764314 (Hartree/Particle)
Thermal correction to Energy=	0.819132
Thermal correction to Enthalpy=	0.820077
Thermal correction to Gibbs Free Energy=	0.669183
Sum of electronic and zero-point Energies=	-3890.363162
Sum of electronic and thermal Energies=	-3890.308343
Sum of electronic and thermal Enthalpies=	-3890.307399
Sum of electronic and thermal Free Energies=	-3890.458293

C

Zero-point correction=	0.765493 (Hartree/Particle)
Thermal correction to Energy=	0.819573
Thermal correction to Enthalpy=	0.820518
Thermal correction to Gibbs Free Energy=	0.672879
Sum of electronic and zero-point Energies=	-3890.355264
Sum of electronic and thermal Energies=	-3890.301184
Sum of electronic and thermal Enthalpies=	-3890.300240
Sum of electronic and thermal Free Energies=	-3890.447878

D

Zero-point correction=	0.766150 (Hartree/Particle)
Thermal correction to Energy=	0.820065
Thermal correction to Enthalpy=	0.821009
Thermal correction to Gibbs Free Energy=	0.672101
Sum of electronic and zero-point Energies=	-3890.395490
Sum of electronic and thermal Energies=	-3890.341576
Sum of electronic and thermal Enthalpies=	-3890.340631
Sum of electronic and thermal Free Energies=	-3890.489539

E

Zero-point correction=	0.765995 (Hartree/Particle)
Thermal correction to Energy=	0.819914
Thermal correction to Enthalpy=	0.820858
Thermal correction to Gibbs Free Energy=	0.671895
Sum of electronic and zero-point Energies=	-3890.395988
Sum of electronic and thermal Energies=	-3890.342069
Sum of electronic and thermal Enthalpies=	-3890.341125
Sum of electronic and thermal Free Energies=	-3890.490088

F

Zero-point correction=	0.498837 (Hartree/Particle)
Thermal correction to Energy=	0.536776
Thermal correction to Enthalpy=	0.537720
Thermal correction to Gibbs Free Energy=	0.425215
Sum of electronic and zero-point Energies=	-3239.979863
Sum of electronic and thermal Energies=	-3239.941924
Sum of electronic and thermal Enthalpies=	-3239.940980
Sum of electronic and thermal Free Energies=	-3240.053485

G

Zero-point correction=	0.497186 (Hartree/Particle)
Thermal correction to Energy=	0.535257
Thermal correction to Enthalpy=	0.536201
Thermal correction to Gibbs Free Energy=	0.423422
Sum of electronic and zero-point Energies=	-3239.972352
Sum of electronic and thermal Energies=	-3239.934282
Sum of electronic and thermal Enthalpies=	-3239.933337
Sum of electronic and thermal Free Energies=	-3240.046116

H

Zero-point correction=	0.497442 (Hartree/Particle)
Thermal correction to Energy=	0.535108
Thermal correction to Enthalpy=	0.536052
Thermal correction to Gibbs Free Energy=	0.424398
Sum of electronic and zero-point Energies=	-3239.992072
Sum of electronic and thermal Energies=	-3239.954405
Sum of electronic and thermal Enthalpies=	-3239.953461
Sum of electronic and thermal Free Energies=	-3240.065115

I

Zero-point correction=	0.778732 (Hartree/Particle)
Thermal correction to Energy=	0.835400
Thermal correction to Enthalpy=	0.836344
Thermal correction to Gibbs Free Energy=	0.675746
Sum of electronic and zero-point Energies=	-4351.278502
Sum of electronic and thermal Energies=	-4351.221833
Sum of electronic and thermal Enthalpies=	-4351.220889
Sum of electronic and thermal Free Energies=	-4351.381488

1

Zero-point correction=	0.499629 (Hartree/Particle)
Thermal correction to Energy=	0.537294
Thermal correction to Enthalpy=	0.538239
Thermal correction to Gibbs Free Energy=	0.424634

Sum of electronic and zero-point Energies=	-3240.071465
Sum of electronic and thermal Energies=	-3240.033799
Sum of electronic and thermal Enthalpies=	-3240.032855
Sum of electronic and thermal Free Energies=	-3240.146460

TS1

Zero-point correction=	0.764999 (Hartree/Particle)
Thermal correction to Energy=	0.818131
Thermal correction to Enthalpy=	0.819075
Thermal correction to Gibbs Free Energy=	0.672990
Sum of electronic and zero-point Energies=	-3890.319585
Sum of electronic and thermal Energies=	-3890.266454
Sum of electronic and thermal Enthalpies=	-3890.265509
Sum of electronic and thermal Free Energies=	-3890.411594

TS2

Zero-point correction=	0.496486 (Hartree/Particle)
Thermal correction to Energy=	0.533916
Thermal correction to Enthalpy=	0.534861
Thermal correction to Gibbs Free Energy=	0.423086
Sum of electronic and zero-point Energies=	-3239.943815
Sum of electronic and thermal Energies=	-3239.906386
Sum of electronic and thermal Enthalpies=	-3239.905441
Sum of electronic and thermal Free Energies=	-3240.017216

TS3

Zero-point correction=	0.497096 (Hartree/Particle)
Thermal correction to Energy=	0.534105
Thermal correction to Enthalpy=	0.535049
Thermal correction to Gibbs Free Energy=	0.424703
Sum of electronic and zero-point Energies=	-3239.971918
Sum of electronic and thermal Energies=	-3239.934909
Sum of electronic and thermal Enthalpies=	-3239.933965
Sum of electronic and thermal Free Energies=	-3240.044311

C'

Zero-point correction=	0.679069 (Hartree/Particle)
Thermal correction to Energy=	0.727335
Thermal correction to Enthalpy=	0.728279
Thermal correction to Gibbs Free Energy=	0.595223
Sum of electronic and zero-point Energies=	-3621.315020
Sum of electronic and thermal Energies=	-3621.266754
Sum of electronic and thermal Enthalpies=	-3621.265810
Sum of electronic and thermal Free Energies=	-3621.398866

H'

Zero-point correction=	0.385401 (Hartree/Particle)
Thermal correction to Energy=	0.415401
Thermal correction to Enthalpy=	0.416345
Thermal correction to Gibbs Free Energy=	0.322016
Sum of electronic and zero-point Energies=	-2509.700888
Sum of electronic and thermal Energies=	-2509.670889
Sum of electronic and thermal Enthalpies=	-2509.669944
Sum of electronic and thermal Free Energies=	-2509.764274

I'

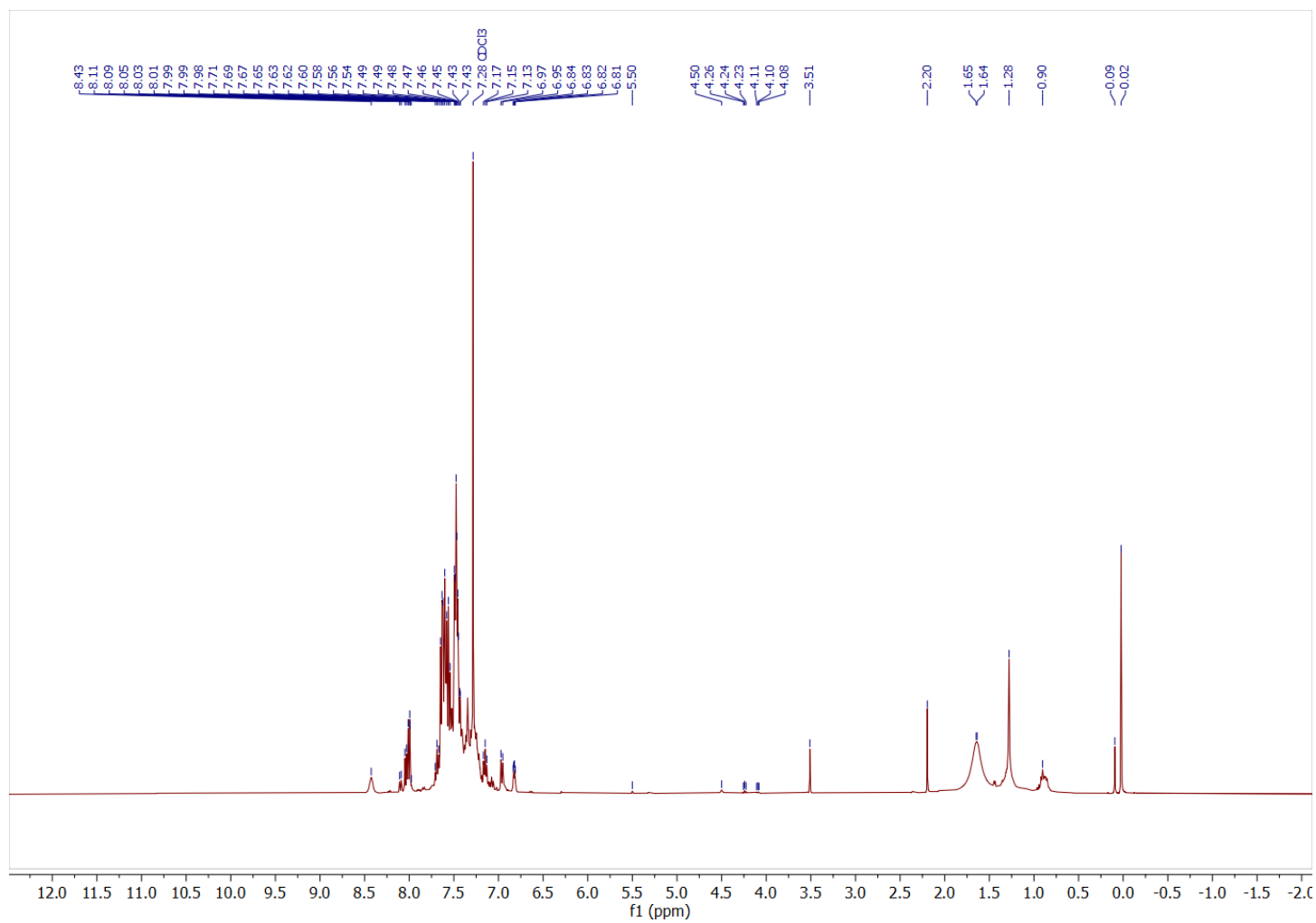
Zero-point correction=	0.679726 (Hartree/Particle)
Thermal correction to Energy=	0.728496
Thermal correction to Enthalpy=	0.729440
Thermal correction to Gibbs Free Energy=	0.591229
Sum of electronic and zero-point Energies=	-3621.417463
Sum of electronic and thermal Energies=	-3621.368694
Sum of electronic and thermal Enthalpies=	-3621.367749
Sum of electronic and thermal Free Energies=	-3621.505960

Table S1: Absolute and relative energies at double zeta (6-31G(d,p) basis) and triple zeta (6-311G(d,p) basis) level of theory

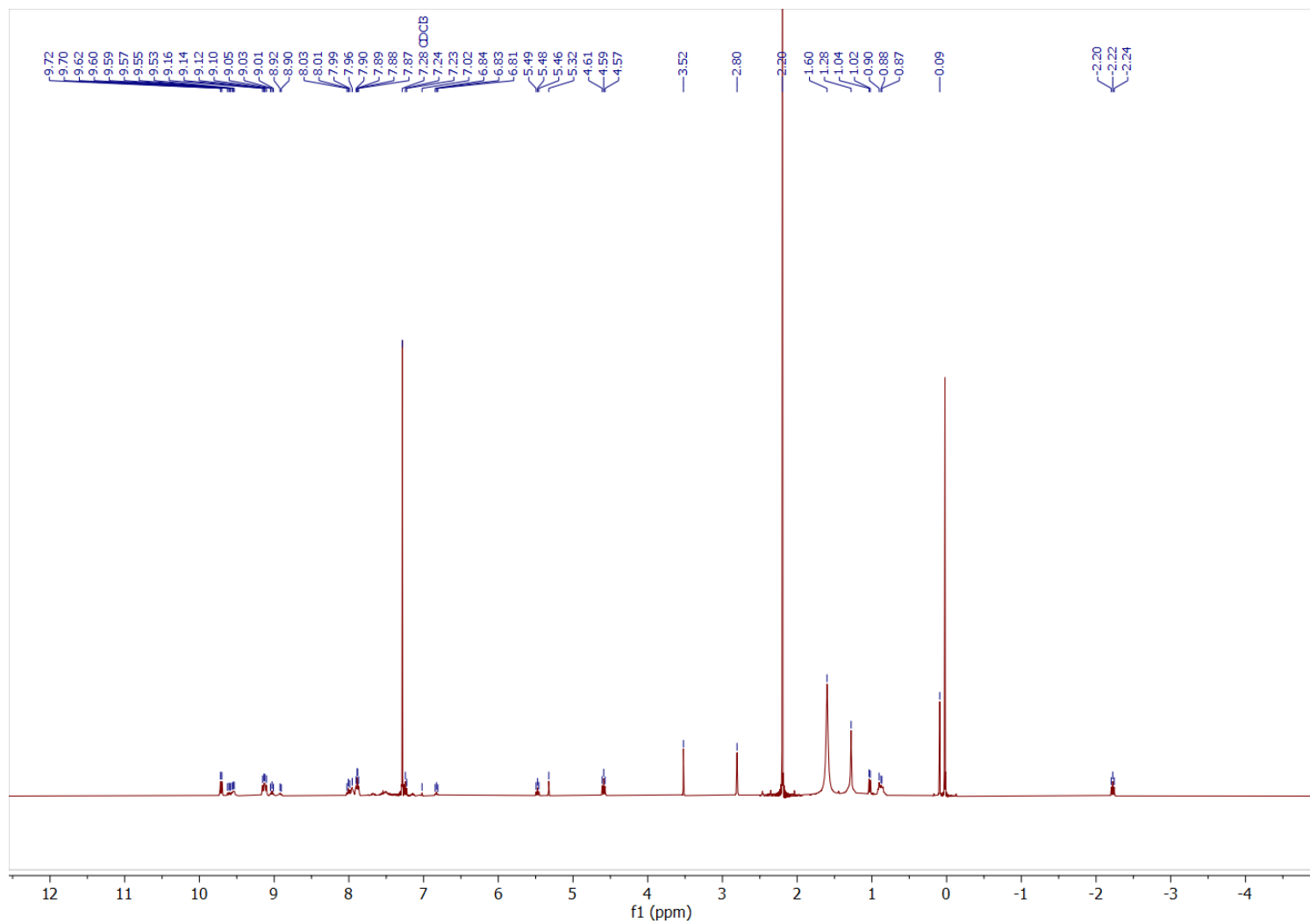
Name	M06L/6-31G(d,p)				M06L/6-311G(d,p)			
	Free Energy (Hartree)	Electronic energy (Hartree)	ΔG kcal/mol	ΔE kcal/mol	Free Energy (Hartree)	Electronic energy (Hartree)	ΔG kcal/mol	ΔE kcal/mol
LNOH	-745.008645	-745.185288			-745.1642799	-745.3409224		
OPPh3	-1111.230167	-1111.461427			-1111.406159	-1111.637418		
HCl	-460.789541	-460.7785827			-460.8163548	-460.8053964		
A	-3606.239584	-3606.719081	0.00	0.00	-3606.663595	-3607.143093	0.00	0.00
B	-3890.458293	-3891.127476	0.25	-1.06	-3891.015963	-3891.685146	-2.79	-4.10
C	-3890.447878	-3891.120757	6.78	3.16	-3891.006558	-3891.679437	3.11	-0.51
TS1	-3890.411594	-3891.084584	29.55	25.85	-3890.96967	-3891.642661	26.26	22.56
D	-3890.489539	-3891.161640	-19.36	-22.50	-3891.049185	-3891.721287	-23.64	-26.77
E	-3890.490088	-3891.161983	-19.70	-22.71	-3891.050454	-3891.722349	-24.43	-27.44
F	-3240.053485	-3240.478701	-22.23	-22.44	-3240.458332	-3240.883547	-22.98	-23.19
TS2	-3240.017216	-3240.440302	0.53	1.66	-3240.41952	-3240.842606	1.38	2.50
G	-3240.046116	-3240.469538	-17.60	-16.69	-3240.448903	-3240.872325	-17.06	-16.14
TS3	-3240.044311	-3240.469014	-16.47	-16.36	-3240.447443	-3240.872146	-16.14	-16.03
H	-3240.065115	-3240.489513	-29.53	-29.22	-3240.467489	-3240.891888	-28.72	-28.42
I	-4351.381488	-4352.057234	-83.62	-95.92	-4351.967034	-4352.642779	-87.32	-99.63
I	-3240.146460	-3240.571094	-80.57	-80.42	-3240.547737	-3240.97237	-79.08	-78.92

2. NMR spectra

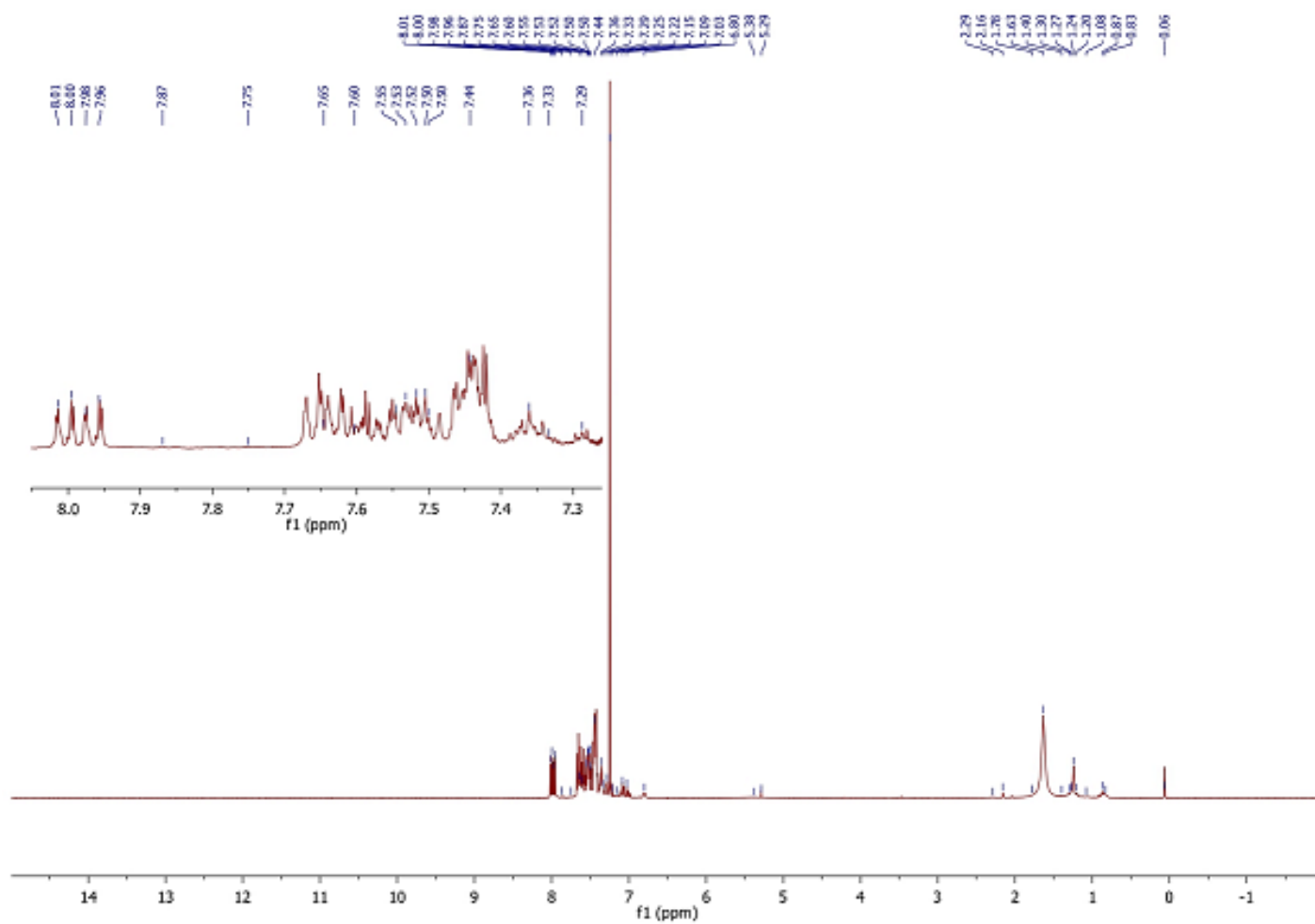
^1H NMR of 1



¹H NMR of 2



¹H NMR of 3



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