Supporting Information

Density Functional Theory Studies on the Mechanism of the isomerization of 2-aryl-2*H*-azirines to 2,3-disubstituted indoles by $FeCl_2$ and $Rh_2(O_2CCF_3)_4$

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Table of Contents

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Cartesian coordinates and electronic energies

2-aryl-2*H*-azirine

E= -634.000918au

C	2.360546	0.214448	−0.932901
C	1.286148	−0.022809	−0.058151
C	3.579950	−0.448261	−0.763323
H	4.395973	−0.258220	−1.453816
C	1.464489	−0.936738	0.997006
H	0.642018	−1.133269	1.679806
C	3.748333	−1.353713	0.290133
C	2.686076	−1.594774	1.170364
H	4.695949	−1.865971	0.424507
H	2.808330	−2.294172	1.992387
C	−0.015602	0.721008	−0.223460
H	2.229532	0.920271	−1.746435
N	−0.000361	1.876011	−1.274959
C	−0.006345	2.183150	−0.052093
C	0.061400	3.363266	0.841425
H	0.974253	3.319973	1.447862
H	0.066878	4.289515	0.258932
H	−0.785863	3.381896	1.535894
C	−1.305313	−0.046294	−0.120742
C	−1.379170	−1.390729	−0.532896
C	−2.481409	0.574065	0.339381
C	−2.588774	−2.089515	−0.482749
H	−0.486517	−1.886251	−0.897734
C	−3.691389	−0.123533	0.391077
H	−2.453037	1.612463	0.654579
C	−3.749965	−1.460447	−0.018791
H	−2.624802	−3.123779	−0.810908
H	−4.585592	0.374997	0.752477
H	−4.688435	−2.004261	0.021476

S-2$_{Fe}$

E= -1019.843498au

N	0.461336	−1.188523	−0.291333
C	−0.870242	−1.351038	−0.505908
C	−1.855757	−0.381565	−0.269371
C	−1.488876	1.039444	−0.170206
C	−0.505887	1.575249	−1.037427
H	−0.139091	0.983489	−1.870134
C	−2.096392	1.898546	0.771583
H	−2.839365	1.501587	1.453047
C	−0.124239	2.923905	−0.941354
H	0.636780	3.302336	−1.614577
C	−0.722258	3.752138	0.009386
H	−0.424557	4.791952	0.093162
C	−1.711392	3.234463	0.860213
H	−2.170576	3.875076	1.606056
C	−3.282397	−0.735939	−0.088646
C	−4.292559	0.041038	−0.700025
C	−3.673836	−1.830632	0.713527
C	−5.640871	−0.282766	−0.536479
H	−4.011228	0.888069	−1.316089
C	−5.023622	−2.141895	0.887882
H	−2.914793	−2.415382	1.220585
C	−6.011938	−1.374116	0.258707
H	−6.401105	0.316510	−1.027052
H	−5.304770	−2.978359	1.519550
H	−7.060409	−1.620470	0.391594
C	−1.209933	−2.768635	−0.963344
H	−0.503309	−3.058391	−1.747925
H	−1.097755	−3.491955	−0.147511
H	−2.224701	−2.842930	−1.359164
Fe	1.385225	0.227208	−0.062006
Cl	2.481684	0.831007	−1.951408
Cl	1.075307	0.980708	1.991585
H	4.078074	0.055718	2.024940
C	4.163409	−0.057834	0.943238
C	5.362563	−0.910206	0.496434
O	2.963202	−0.820954	0.519157
H	4.133348	0.921094	0.461063

C	4.762053	-2.322681	0.307474
H	6.172114	-0.890633	1.231658
H	5.757198	-0.539784	-0.455716
C	3.366879	-2.021344	-0.235933
H	5.347960	-2.938447	-0.381353
H	4.695310	-2.847623	1.267194
H	2.609379	-2.775249	-0.031402
H	3.373597	-1.772655	-1.301213

S'-2$_{Fe}$

E= -1019.8751802au

N	0.425067	-1.206231	-0.271622
C	-0.911436	-1.362917	-0.502238
C	-1.891896	-0.378246	-0.261140
C	-1.461790	1.027800	-0.177886
C	-0.414668	1.491241	-1.032556
H	-0.107221	0.882441	-1.887633
C	-2.048200	1.946184	0.729130
H	-2.834248	1.604408	1.403822
C	0.038832	2.830407	-0.953053
H	0.838586	3.153147	-1.621666
C	-0.541560	3.716153	-0.035356
H	-0.186651	4.745972	0.037716
C	-1.588029	3.268177	0.798885
H	-2.035095	3.953974	1.522334
C	-3.324784	-0.698279	-0.075076
C	-4.327699	0.121367	-0.663081
C	-3.742806	-1.810891	0.704245
C	-5.688735	-0.175160	-0.496573
H	-4.027279	0.979652	-1.267472
C	-5.105194	-2.097919	0.876096
H	-2.990086	-2.425738	1.200656
C	-6.084420	-1.285648	0.272846
H	-6.442051	0.459618	-0.968966
H	-5.404302	-2.950336	1.490501
H	-7.144554	-1.512380	0.406052
C	-1.251768	-2.776892	-0.977421
H	-0.555537	-3.054875	-1.785426
H	-1.123608	-3.518288	-0.171612
H	-2.280864	-2.840823	-1.356928
Fe	1.361759	0.217614	-0.071404
Cl	2.528685	0.784706	-1.922409
Cl	1.092335	1.027830	1.956634
H	4.065016	0.048653	2.048503
C	4.139790	-0.079574	0.960520
C	5.334067	-0.940923	0.505659
O	2.917707	-0.856193	0.571382
H	4.097103	0.897783	0.460117
C	4.725703	-2.356710	0.326144
H	6.154872	-0.922567	1.238798
H	5.723718	-0.573607	-0.457472
C	3.328520	-2.048720	-0.216816
H	5.310546	-2.980793	-0.367083
H	4.658751	-2.880437	1.294235
H	2.561263	-2.806061	-0.023883
H	3.337869	-1.774368	-1.283583

T-2$_{Fe}$

E= -1019.9059205au

N	0.219975	-0.895945	-0.598660
C	-1.029940	-1.199706	-0.723108
C	-2.113850	-0.310073	-0.362234
C	-1.890143	1.131526	-0.231863
C	-0.918449	1.810620	-1.009568
H	-0.342052	1.272321	-1.754038
C	-2.653390	1.893007	0.690246
H	-3.388614	1.394096	1.310510
C	-0.705839	3.180348	-0.853722
H	0.059405	3.666889	-1.448447
C	-1.460460	3.910348	0.072996
H	-1.286752	4.973871	0.200003
C	-2.435923	3.260350	0.841577
H	-3.013995	3.817810	1.571302
C	-3.463361	-0.862534	-0.123736
C	-4.600214	-0.229668	-0.678872
C	-3.661989	-2.014825	0.670049
C	-5.880488	-0.742708	-0.463575
H	-4.466624	0.657075	-1.288557

C	-4.945097	-2.518432	0.892351
H	-2.808841	-2.490847	1.141195
C	-6.058712	-1.888610	0.322185
H	-6.738659	-0.249471	-0.908558
H	-5.077278	-3.395415	1.517783
H	-7.055030	-2.283089	0.493175
C	-1.295572	-2.592435	-1.312787
H	-0.494352	-2.848936	-2.010540
H	-1.313676	-3.354665	-0.528031
H	-2.251982	-2.611541	-1.838739
Fe	1.749310	0.230670	0.082725
Cl	2.698098	1.505836	-1.546744
Cl	1.233078	0.731931	2.223816
H	4.289736	-1.938609	2.008792
C	4.294524	-1.029258	1.395394
C	5.624695	-0.824931	0.673123
O	3.322733	-1.207947	0.302294
H	3.945370	-0.186845	1.992956
C	5.509979	-1.808438	-0.514871
H	6.486525	-1.034522	1.313203
H	5.699673	0.206544	0.312262
C	4.014728	-1.756289	-0.884719
H	6.145291	-1.521980	-1.357478
H	5.798507	-2.818398	-0.201353
H	3.586004	-2.739393	-1.098933
H	3.810622	-1.068921	-1.708513

T'-2$_{Fe}$

E= -1019.9043677au

N	0.316263	-0.717657	-0.961735
C	-0.974710	-1.023808	-0.988091
C	-2.029541	-0.238502	-0.417628
C	-1.863631	1.187994	-0.106110
C	-1.029357	2.030106	-0.891904
H	-0.491845	1.615814	-1.746295
C	-2.572729	1.771599	0.984181
H	-3.196983	1.136382	1.614210
C	-0.906529	3.393559	-0.595263
H	-0.252230	4.016700	-1.207366
C	-1.607525	3.950605	0.490971
H	-1.502708	5.012680	0.724004
C	-2.439792	3.132996	1.280442
H	-2.973562	3.555783	2.134422
C	-3.351055	-0.860580	-0.166249
C	-4.548341	-0.188009	-0.536039
C	-3.460240	-2.126896	0.469418
C	-5.801701	-0.772387	-0.300112
H	-4.481153	0.785631	-1.024896
C	-4.716292	-2.700167	0.717379
H	-2.553466	-2.636770	0.799983
C	-5.891488	-2.029384	0.327948
H	-6.709417	-0.247312	-0.606044
H	-4.779742	-3.666374	1.222999
H	-6.868489	-2.479645	0.517179
C	-1.262487	-2.329624	-1.748176
H	-0.602644	-2.382234	-2.627591
H	-1.047109	-3.210846	-1.122492
H	-2.308855	-2.378276	-2.078611
Fe	1.652938	0.027694	-0.182980
Cl	2.510697	1.818486	-1.241307
Cl	1.057192	0.085374	1.974332
H	3.890785	-2.493199	1.484921
C	4.029124	-1.404040	1.366956
C	5.502397	-1.016887	1.217753
O	3.422958	-1.005090	0.070149
H	3.467777	-0.870803	2.144067
C	5.791335	-1.357644	-0.266865
H	6.152566	-1.569038	1.913563
H	5.632016	0.062261	1.401631
C	4.479766	-0.982276	-0.984139
H	6.649287	-0.797546	-0.668649
H	6.005525	-2.434209	-0.376029
H	4.180274	-1.698293	-1.764256
H	4.478733	0.038029	-1.394559

Q'-2$_{Fe}$

E= -1019.915029au

N	0.309514	-0.443213	-0.324683

C	-0.865072	-0.989668	-0.542169
C	-2.100750	-0.294803	-0.242449
C	-2.125159	1.159216	-0.041371
C	-1.241938	2.027329	-0.745171
H	-0.549073	1.617855	-1.481084
C	-3.047409	1.742285	0.878579
H	-3.718414	1.093835	1.444060
C	-1.272409	3.410418	-0.526087
H	-0.579731	4.052044	-1.073879
C	-2.179622	3.965010	0.397147
H	-2.194090	5.043377	0.570956
C	-3.067528	3.124859	1.097768
H	-3.765551	3.548122	1.823398
C	-3.372019	-1.040309	-0.113841
C	-4.565339	-0.533864	-0.701221
C	-3.448288	-2.259425	0.614197
C	-5.776700	-1.230828	-0.582511
H	-4.523401	0.398818	-1.266606
C	-4.665696	-2.943319	0.745264
H	-2.553095	-2.644489	1.105796
C	-5.833165	-2.436410	0.142520
H	-6.677771	-0.833446	-1.054994
H	-4.706835	-3.868364	1.324732
H	-6.778900	-2.973781	0.241172
C	-0.876824	-2.403309	-1.145691
H	-0.118921	-2.443348	-1.943217
H	-0.602064	-3.161932	-0.393917
H	-1.855231	-2.671286	-1.567507
Fe	1.832467	0.459164	-0.022526
Cl	2.346197	2.005854	-1.566786
Cl	2.313407	0.957627	2.112616
H	3.129215	-2.945444	-0.836350
C	3.351464	-2.344728	0.060300
C	4.742975	-2.643405	0.643860
O	3.403427	-0.924387	-0.375788
H	2.533245	-2.445913	0.786576
C	5.661789	-1.650243	-0.112681
H	5.036221	-3.693966	0.495648
H	4.760230	-2.429164	1.725038
C	4.785501	-0.396136	-0.204629
H	6.604704	-1.457316	0.421067
H	5.905041	-2.032565	-1.118323
H	4.976358	0.250862	-1.070377
H	4.803782	0.200225	0.722588

Sep-2$_{Fe}$

E= -1019.9120932au

N	0.297342	-0.414976	-0.333423
C	-0.852147	-0.958575	-0.531852
C	-2.112114	-0.274983	-0.258237
C	-2.168979	1.179272	-0.108091
C	-1.257402	2.043830	-0.767577
H	-0.506686	1.637510	-1.434462
C	-3.160315	1.772507	0.719432
H	-3.859398	1.135725	1.248618
C	-1.324429	3.425414	-0.591457
H	-0.605665	4.057837	-1.101708
C	-2.301970	3.987632	0.239589
H	-2.346934	5.062834	0.379637
C	-3.220240	3.153146	0.892328
H	-3.973968	3.579780	1.546358
C	-3.355194	-1.065806	-0.124913
C	-4.529717	-0.667783	-0.805447
C	-3.416623	-2.219631	0.688874
C	-5.709146	-1.406031	-0.690973
H	-4.502021	0.216810	-1.432239
C	-4.600825	-2.949836	0.809823
H	-2.540040	-2.520564	1.252704
C	-5.750162	-2.549982	0.116460
H	-6.595580	-1.089786	-1.231476
H	-4.629866	-3.824510	1.451808
H	-6.668838	-3.120146	0.208905
C	-0.849437	-2.381218	-1.105632
H	0.054417	-2.522724	-1.703228
H	-0.847526	-3.129886	-0.306669
H	-1.727404	-2.555608	-1.731499
Fe	1.915976	0.563407	0.133562
Cl	2.406330	2.189400	-1.342661

Cl	2.189139	0.706701	2.356784
H	2.858748	-2.782037	-0.838035
C	3.328847	-2.287726	0.017244
C	4.779323	-2.744579	0.250344
O	3.415756	-0.853752	-0.314499
H	2.695323	-2.396818	0.900519
C	5.617971	-1.690812	-0.509379
H	4.951347	-3.762306	-0.111318
H	5.019644	-2.719204	1.318787
C	4.821486	-0.407544	-0.277816
H	6.641591	-1.617339	-0.131470
H	5.662264	-1.926746	-1.578673
H	4.924138	0.353241	-1.052061
H	5.017124	0.032693	0.706441

Sep'-2$_{Fe}$

E= -1019.9051076au

N	0.307804	-0.469259	-0.484182
C	-0.871318	-0.966129	-0.683727
C	-2.112932	-0.264033	-0.311681
C	-2.123487	1.186191	-0.109354
C	-1.224139	2.053270	-0.798837
H	-0.524994	1.640129	-1.526746
C	-3.050496	1.782444	0.800597
H	-3.732137	1.140807	1.360912
C	-1.245740	3.436340	-0.579867
H	-0.539742	4.072014	-1.117966
C	-2.162029	4.000964	0.328440
H	-2.170418	5.079352	0.502053
C	-3.064520	3.165125	1.016199
H	-3.768809	3.592582	1.733662
C	-3.361381	-1.031616	-0.128649
C	-4.592113	-0.547214	-0.657633
C	-3.383505	-2.262655	0.584997
C	-5.782393	-1.270126	-0.493655
H	-4.594930	0.391811	-1.214313
C	-4.578250	-2.977705	0.754387
H	-2.461625	-2.633782	1.037315
C	-5.782414	-2.488743	0.212470
H	-6.711500	-0.885127	-0.920426
H	-4.573192	-3.912581	1.319796
H	-6.711076	-3.048700	0.342893
C	-0.949686	-2.337963	-1.376287
H	-0.165000	-2.387433	-2.145898
H	-0.765007	-3.155955	-0.660563
H	-1.929943	-2.503745	-1.843458
Fe	1.847306	0.491168	0.039157
Cl	2.454843	2.190970	-1.275725
Cl	2.120917	0.625668	2.252395
H	3.005274	-2.850087	-0.894580
C	3.334917	-2.305837	0.003701
C	4.756541	-2.691649	0.455474
O	3.414466	-0.869841	-0.379828
H	2.581210	-2.404529	0.797645
C	5.657739	-1.645078	-0.249593
H	5.010078	-3.726067	0.177859
H	4.850512	-2.597473	1.549645
C	4.802329	-0.376372	-0.180021
H	6.629094	-1.519573	0.252287
H	5.843464	-1.930768	-1.298404
H	4.981057	0.360062	-0.973659
H	4.856701	0.114079	0.806612

Sep-TS$_{(2-3)Fe}$

E= -1019.8750678au

C	-1.016805	-0.689101	0.161421
N	0.047913	0.102531	0.068753
C	-2.269009	-0.110445	-0.202830
C	-2.050381	1.314148	-0.506261
C	-0.702195	1.571175	-0.982133
H	-0.350384	0.999976	-1.842052
C	-2.837551	2.357190	-0.035361
H	-3.822382	2.145878	0.367920
C	-0.192508	2.907349	-0.871105
H	0.812866	3.121285	-1.212894
C	-0.995683	3.926019	-0.362241
H	-0.597835	4.932700	-0.287617
C	-2.325303	3.673094	0.012202

H	−2.949731	4.479157	0.382311
C	−0.823999	−2.118561	0.622234
H	0.189208	−2.454494	0.397207
H	−0.941381	−2.199622	1.708941
H	−1.541784	−2.788188	0.140859
C	−3.594865	−0.723212	−0.167610
C	−4.576241	−0.288067	−1.095541
C	−3.966119	−1.726011	0.761780
C	−5.852336	−0.849120	−1.111430
H	−4.315548	0.481449	−1.814085
C	−5.247918	−2.278266	0.745816
H	−3.264021	−2.044190	1.521344
C	−6.195429	−1.849937	−0.192426
H	−6.580201	−0.507962	−1.840721
H	−5.511513	−3.037286	1.475463
H	−7.189858	−2.283954	−0.202237
Cl	2.910359	2.305849	0.612215
Fe	1.941477	0.265917	0.804038
Cl	2.153290	−1.177869	2.529386
H	2.359896	−2.681432	−0.472672
C	2.735091	−2.048152	−1.280992
C	4.039659	−2.588505	−1.901916
O	3.071490	−0.728947	−0.721586
H	1.943680	−1.884392	−2.017784
C	4.936746	−1.334819	−2.027994
H	3.863179	−3.077828	−2.863956
H	4.505343	−3.320371	−1.233045
C	4.525340	−0.509289	−0.810131
H	6.002581	−1.580292	−2.023901
H	4.714168	−0.787344	−2.950852
H	4.668884	0.567061	−0.899549
H	4.994169	−0.868724	0.113649

S-$FeCl_2$(THF)

E= -385.783951au

Cl	−1.619178	−2.136047	0.115330
Fe	−1.094422	0.000121	−0.000007
Cl	−1.618157	2.136555	−0.115611
H	1.597168	1.196985	1.528219
C	1.675747	1.147007	0.439161
C	3.078022	0.772582	−0.038750
O	0.824195	−0.000250	0.000531
H	1.238781	2.039999	−0.006243
C	3.078294	−0.772899	0.037702
H	3.852729	1.222847	0.587682
H	3.237071	1.106696	−1.069937
C	1.675379	−1.147857	−0.438047
H	3.852165	−1.222947	−0.589918
H	3.239073	−1.106920	1.068648
H	1.239165	−2.040512	0.008773
H	1.595316	−1.198911	−1.526929

T-$FeCl_2$(THF)

E= -385.8548131au

Cl	−1.592871	2.154038	−0.007386
Fe	−1.128929	0.008310	−0.007717
Cl	−1.687051	−2.111037	0.029678
H	1.642692	−1.526750	−1.243261
C	1.696802	−1.227379	−0.192876
C	3.100405	−0.785494	0.224483
O	0.867926	−0.001675	−0.041765
H	1.246338	−1.999035	0.430455
C	3.135662	0.705095	−0.183145
H	3.876289	−1.375882	−0.270439
H	3.231874	−0.889852	1.307291
C	1.729503	1.193396	0.167264
H	3.906317	1.269095	0.349379
H	3.322035	0.805049	−1.258319
H	1.335947	1.984237	−0.470100
H	1.631699	1.485754	1.216434

Sep-$FeCl_2$(THF)

E= -385.7570257au

Cl	−1.680614	−1.765715	−0.536466
Fe	−1.060791	−0.019179	0.732234
Cl	−1.746795	1.755218	−0.462097
H	1.816598	1.616693	1.106136
C	1.741118	1.237322	0.082389

C	3.079510	0.746612	-0.472310
O	0.900482	0.013539	0.124917
H	1.216152	1.958843	-0.543930
C	3.171805	-0.702559	0.058344
H	3.911840	1.370980	-0.135465
H	3.067238	0.755394	-1.567672
C	1.730796	-1.209277	-0.039527
H	3.858422	-1.320976	-0.526302
H	3.511142	-0.707832	1.100020
H	1.439983	-1.906347	0.748371
H	1.481917	-1.630535	-1.016397

$FeCl_2(THF)$

E= -385.898783au

Cl	-1.758894	-2.097814	0.033629
Fe	-1.102151	0.000113	0.000018
Cl	-1.757301	2.098592	-0.034526
H	1.725821	1.459652	1.282361
C	1.795324	1.200592	0.221760
C	3.201117	0.751704	-0.182001
O	0.949761	-0.000353	0.001117
H	1.374274	2.006645	-0.379641
C	3.202807	-0.751523	0.177927
H	3.975991	1.312937	0.347219
H	3.355867	0.889014	-1.258067
C	1.794854	-1.202234	-0.217203
H	3.974920	-1.312069	-0.356029
H	3.364491	-0.888645	1.252989
H	1.377127	-2.005573	0.390167
H	1.720048	-1.466532	-1.276074

$\mathbf{1}_{Fe}$

E= -1019.9314736au

C	1.080874	2.213645	-0.929043
C	1.579638	1.781780	0.314554
C	1.074844	3.574390	-1.249216
H	0.686190	3.899523	-2.208995
C	2.077175	2.728520	1.222067
H	2.471041	2.399138	2.181081
C	1.572370	4.514996	-0.337315
C	2.074778	4.091282	0.897755
H	1.569296	5.570740	-0.589699
H	2.463474	4.816501	1.606317
C	1.564580	0.314281	0.649840
H	0.693608	1.481821	-1.632331
N	0.161271	-0.291484	0.825205
C	0.861973	-0.153938	1.867348
C	0.838489	-0.490309	3.305036
H	0.833256	0.421794	3.914085
H	-0.043613	-1.092558	3.539475
H	1.739752	-1.053673	3.571945
C	2.594465	-0.586656	0.020426
C	3.746382	-0.047002	-0.580669
C	2.432470	-1.986547	0.041540
C	4.709532	-0.885073	-1.150144
H	3.885925	1.027445	-0.608749
C	3.394144	-2.819517	-0.536574
H	1.549575	-2.430397	0.489544
C	4.536836	-2.273466	-1.132311
H	5.590725	-0.451678	-1.612538
H	3.244951	-3.894235	-0.525170
H	5.281579	-2.922562	-1.581418
Cl	-1.171895	-1.088024	-2.384027
Fe	-1.417695	-1.334534	-0.149089
Cl	-1.660363	-3.077071	1.266986
H	-1.967436	1.863117	0.068107
C	-2.809449	1.438623	0.624029
C	-4.133858	2.138754	0.296941
O	-2.992933	0.045077	0.182528
H	-2.569909	1.416622	1.689484
C	-4.635030	1.360475	-0.939724
H	-3.996098	3.205536	0.098827
H	-4.841540	2.034450	1.127458
C	-4.225258	-0.080507	-0.624217
H	-5.713203	1.459245	-1.093803
H	-4.125123	1.709193	-1.844541
H	-3.972435	-0.670775	-1.506754
H	-4.966723	-0.607359	-0.014921

$\mathbf{2}_{Fe}$

E= -1019.9143482au

N	0.312598	−0.428770	−0.271783
C	−0.842198	−0.982744	−0.476532
C	−2.093014	−0.293913	−0.226301
C	−2.138341	1.162432	−0.074229
C	−1.252378	2.017951	−0.776078
H	−0.536529	1.603662	−1.475391
C	−3.086961	1.759024	0.798018
H	−3.765145	1.125473	1.357617
C	−1.303365	3.400178	−0.598496
H	−0.605849	4.028755	−1.141643
C	−2.236342	3.967171	0.279094
H	−2.267271	5.042628	0.421343
C	−3.128750	3.140012	0.975319
H	−3.847415	3.572111	1.664108
C	−3.352366	−1.057493	−0.106824
C	−4.526656	−0.600397	−0.750862
C	−3.432699	−2.241730	0.661476
C	−5.723535	−1.311059	−0.646773
H	−4.484417	0.306283	−1.343958
C	−4.635051	−2.941843	0.775353
H	−2.555535	−2.590943	1.194868
C	−5.783607	−2.483514	0.117280
H	−6.608816	−0.950750	−1.160738
H	−4.678646	−3.839913	1.383133
H	−6.716230	−3.031614	0.203057
C	−0.828128	−2.416139	−1.022078
H	0.003973	−2.511813	−1.725017
H	−0.668349	−3.143744	−0.218341
H	−1.759356	−2.669556	−1.532210
Fe	1.857869	0.512072	0.060073
Cl	2.357164	2.066524	−1.493358
Cl	2.298088	0.951800	2.220608
H	2.980580	−2.820900	−0.953139
C	3.297855	−2.330298	−0.027484
C	4.711081	−2.743756	0.406363
O	3.386325	−0.886875	−0.309061
H	2.540275	−2.478648	0.744548
C	5.614345	−1.706309	−0.298686
H	4.943661	−3.773360	0.119763
H	4.816163	−2.660147	1.493681
C	4.786571	−0.423951	−0.203313
H	6.590363	−1.602636	0.183631
H	5.777673	−1.984292	−1.346239
H	4.939955	0.289808	−1.013403
H	4.899481	0.078843	0.762655

$\mathbf{TS}_{(2\text{-}3)Fe}$

E= -1019.8967373au

C	0.983024	−0.750507	−0.177527
N	−0.093109	−0.032588	−0.316074
C	2.229052	−0.075702	0.157575
C	2.056167	1.304397	0.456434
C	0.722955	1.750829	0.760703
H	0.092870	1.142125	1.401913
C	3.062097	2.289003	0.201100
H	4.074924	1.967017	−0.010528
C	0.379776	3.115150	0.596542
H	−0.643045	3.430565	0.765795
C	1.363232	4.032726	0.265578
H	1.110031	5.082668	0.160282
C	2.714270	3.621871	0.101939
H	3.470337	4.360352	−0.143370
C	0.871602	−2.267343	−0.288272
H	0.420212	−2.662124	0.630829
H	0.209424	−2.535252	−1.115336
H	1.842357	−2.746717	−0.418346
C	3.550862	−0.729691	0.174006
C	4.427657	−0.532949	1.264269
C	3.993441	−1.522476	−0.909007
C	5.694380	−1.120894	1.278450
H	4.098399	0.070957	2.103455
C	5.263622	−2.102466	−0.895334
H	3.350552	−1.651860	−1.773029
C	6.115570	−1.908318	0.199565
H	6.350388	−0.968130	2.129273

H	5.591525	-2.698632	-1.740559
H	7.100361	-2.363959	0.209797
Cl	-2.614136	2.099420	-1.458665
Fe	-1.937234	0.008361	-0.906844
Cl	-2.492387	-1.935582	-1.941828
H	-2.432121	-2.274225	1.104893
C	-2.904239	-1.505296	1.720324
C	-4.317959	-1.888890	2.187636
O	-3.073761	-0.297195	0.890791
H	-2.245257	-1.233709	2.551485
C	-5.097718	-0.557950	2.094594
H	-4.316939	-2.311466	3.196544
H	-4.753578	-2.629827	1.508517
C	-4.499111	0.084338	0.843465
H	-6.177589	-0.707895	2.006830
H	-4.908254	0.065295	2.976321
H	-4.530394	1.173249	0.812054
H	-4.935449	-0.320375	-0.076566

$TS_{(2\text{-}4)Fe}$

E= -1019.8750217au

C	0.898199	-0.782961	-0.258572
N	-0.259232	-0.206532	-0.504113
C	2.112478	-0.009649	-0.107237
C	2.045451	1.435747	-0.238743
C	0.808565	2.046634	-0.504070
H	-0.100436	0.934249	-0.597820
C	3.168308	2.307848	-0.169347
H	4.156098	1.896058	0.003071
C	0.611021	3.394979	-0.704071
H	-0.370840	3.797055	-0.930836
C	1.741552	4.234303	-0.606921
H	1.630799	5.305310	-0.745367
C	3.003877	3.682630	-0.342939
H	3.871093	4.332429	-0.285654
C	3.401216	-0.678997	0.206950
C	4.072561	-0.403393	1.417349
C	3.990837	-1.587076	-0.696474
C	5.286615	-1.027492	1.718613
H	3.629756	0.291077	2.124149
C	5.208592	-2.203336	-0.396448
H	3.501558	-1.791646	-1.642991
C	5.858437	-1.928917	0.812982
H	5.783712	-0.811516	2.658951
H	5.651147	-2.893239	-1.107692
H	6.802121	-2.411154	1.046274
C	0.909357	-2.291970	-0.092411
H	1.450903	-2.582730	0.813079
H	-0.111805	-2.674412	-0.053357
H	1.406209	-2.774666	-0.940518
Cl	-2.951766	1.300445	-1.815940
Fe	-2.195176	-0.629107	-0.895271
Cl	-2.584421	-2.771530	-1.436896
H	-1.840520	1.114359	1.890665
C	-2.306680	0.176257	2.210097
O	-2.999536	-0.409296	1.052991
C	-3.404763	0.399688	3.255611
H	-1.532153	-0.528228	2.520152
C	-4.463755	-0.266996	1.198863
C	-4.650429	0.682882	2.386268
H	-3.165907	1.223439	3.934374
H	-3.554156	-0.505190	3.855735
H	-4.872070	-1.265189	1.383486
H	-4.845721	0.125723	0.254650
H	-5.588046	0.498574	2.918091
H	-4.649743	1.723952	2.044687

3_{Fe}

E= -1019.9538821au

N	-0.076140	-0.133499	0.238592
C	-1.199005	-0.792359	0.039943
C	-2.372265	0.091801	-0.012245
C	-1.899435	1.372246	0.164665
C	-0.427620	1.274140	0.437421
H	-0.279260	1.403745	1.533956
C	0.392815	2.388657	-0.147882
C	-2.489136	2.675330	0.003222
H	-3.567003	2.787686	-0.024646

C	−0.219880	3.574110	−0.384984
C	−1.662667	3.734577	−0.249782
H	−2.086591	4.718051	−0.426986
H	1.464606	2.251399	−0.239376
H	0.360796	4.434007	−0.703840
C	−3.777815	−0.327791	−0.200673
C	−4.779090	0.156761	0.666468
C	−4.157061	−1.193103	−1.246670
C	−6.115874	−0.210703	0.491148
H	−4.497549	0.803809	1.491113
C	−5.494229	−1.560334	−1.419437
H	−3.406751	−1.559441	−1.938884
C	−6.478166	−1.071056	−0.552002
H	−6.871621	0.166567	1.172720
H	−5.768405	−2.223438	−2.233785
H	−7.515713	−1.359164	−0.686408
C	−1.244141	−2.286152	−0.073247
H	−2.035888	−2.698278	0.561352
H	−1.467799	−2.593042	−1.102212
H	−0.285550	−2.730540	0.202448
Cl	2.421728	−2.920277	0.243461
Fe	1.869442	−0.799206	0.834713
Cl	2.170480	0.435552	2.723566
H	6.209107	0.830615	−1.532448
C	5.123541	0.963864	−1.535465
C	4.478825	0.501417	−0.229935
C	4.419439	0.073652	−2.586067
H	4.908848	2.023677	−1.715369
O	3.072465	0.252100	−0.599365
H	4.463245	1.237118	0.574437
H	4.915007	−0.435454	0.135457
C	2.987861	−0.076563	−2.039384
H	4.431769	0.513256	−3.587429
H	4.909151	−0.904524	−2.639556
H	2.600235	−1.093811	−2.127731
H	2.282986	0.634162	−2.480602

$TS_{(3\text{-}4)Fe}$

E= -1019.921179au

N	−0.066632	−0.169559	0.347641
C	−1.269332	−0.824442	0.176996
C	−2.334485	0.075982	0.002954
C	−1.808252	1.390828	0.129879
C	−0.394346	1.257182	0.362990
H	−0.141960	0.641993	1.437786
C	0.487236	2.386008	0.287555
C	−2.358483	2.691415	−0.010190
H	−3.422771	2.818604	−0.171949
C	−0.096328	3.628506	0.155724
C	−1.509193	3.782144	0.016113
H	−1.916402	4.781571	−0.096671
H	1.557587	2.251234	0.386845
H	0.530405	4.514205	0.148097
C	−3.757523	−0.266983	−0.222576
C	−4.766708	0.311336	0.573466
C	−4.135160	−1.159078	−1.245705
C	−6.112313	0.002491	0.354800
H	−4.489823	0.987088	1.376397
C	−5.481343	−1.468561	−1.460841
H	−3.371288	−1.592052	−1.883412
C	−6.474126	−0.889011	−0.662051
H	−6.876248	0.451555	0.981646
H	−5.754717	−2.155545	−2.255440
H	−7.518923	−1.129208	−0.830630
C	−1.322053	−2.317650	0.310533
H	−1.017314	−2.623584	1.320009
H	−2.334006	−2.688273	0.138330
H	−0.637218	−2.809756	−0.387766
Fe	1.907354	−1.007777	0.696413
Cl	2.309082	−2.908188	−0.455015
Cl	2.177174	−0.205123	2.805980
O	3.046618	0.351852	−0.494575
C	4.483843	0.479462	−0.183698
C	2.841881	0.431338	−1.959336
C	5.055645	1.235490	−1.382223
H	4.551412	0.998027	0.773252
H	4.910935	−0.525664	−0.090936

C	4.240151	0.653795	-2.560214
H	2.377349	-0.502540	-2.282855
H	2.162056	1.270389	-2.134313
H	6.131615	1.076846	-1.497212
H	4.876911	2.311999	-1.278638
H	4.212425	1.322364	-3.425198
H	4.671247	-0.300194	-2.882428

$\mathbf{4_{Fe}}$

E= -1019.9963159au

C	1.267887	-1.195318	-0.817217
N	-0.011006	-0.784338	-1.335399
C	2.027639	-0.085914	-0.552528
C	1.271121	1.087723	-0.987302
C	0.051818	0.623406	-1.526629
H	-0.392675	-1.327341	-2.109751
C	1.550861	2.464771	-1.010289
H	2.484393	2.844790	-0.610358
C	-0.888450	1.473893	-2.109666
H	-1.814413	1.088777	-2.523119
C	-0.587113	2.840979	-2.130958
H	-1.289820	3.533737	-2.582640
C	0.614645	3.330280	-1.581892
H	0.821207	4.395206	-1.616391
C	3.379413	-0.050617	0.052376
C	3.643892	0.786187	1.155286
C	4.432461	-0.829179	-0.466809
C	4.917986	0.832572	1.727972
H	2.840963	1.385503	1.572470
C	5.705731	-0.784317	0.109298
H	4.253601	-1.452613	-1.336631
C	5.953047	0.045987	1.208360
H	5.101277	1.477032	2.582058
H	6.505287	-1.390121	-0.305463
H	6.942173	0.082143	1.653464
C	1.529494	-2.649804	-0.592868
H	2.511205	-2.793177	-0.137482
H	0.780098	-3.084747	0.079263
H	1.507410	-3.217536	-1.533618
Cl	-3.127122	-1.660918	-1.836027
Fe	-1.864197	-1.295441	0.013181
Cl	-1.266314	-2.399256	1.873014
H	-1.036328	2.062550	0.948352
C	-1.623135	1.434821	1.623873
O	-2.462634	0.558183	0.777728
C	-2.616324	2.239299	2.474485
H	-0.963744	0.791213	2.210244
C	-3.892071	0.854085	0.988169
C	-3.897282	2.251421	1.609276
H	-2.245772	3.244670	2.693232
H	-2.806415	1.732142	3.426896
H	-4.305357	0.099162	1.666890
H	-4.377982	0.779374	0.014328
H	-4.800777	2.439233	2.196154
H	-3.828424	3.017681	0.828968

$\mathbf{Rh_2(OCOCF_3)_4}$

E= -2323.3500744au

Rh	-0.004786	-0.001644	1.210990
O	-1.420991	-1.499930	1.147285
C	-1.816517	-1.920400	-0.000517
C	-2.918876	-2.978747	0.000594
Rh	0.000884	-0.002693	-1.205257
O	1.494545	-1.417969	1.154610
O	1.412345	1.496648	1.152053
O	-1.502696	1.414907	1.145937
O	-1.418720	-1.498413	-1.146581
O	1.419485	1.493213	-1.141778
O	-1.495217	1.416598	-1.147899
O	1.497459	-1.420267	-1.139220
C	1.918706	-1.814206	0.009035
C	1.812458	1.916332	0.005806
C	-1.920167	1.812475	-0.002051
C	2.988352	-2.905660	-0.002370
C	2.914088	2.975448	0.003559
C	-2.978139	2.915179	-0.006650
F	2.871116	3.740108	1.146036
F	4.146471	2.342203	-0.054624

F	2.799441	3.805440	−1.088265
F	−3.760417	2.857768	1.123408
F	−3.791206	2.816524	−1.112442
F	−2.342646	4.147422	−0.038204
F	−2.865146	−3.753532	−1.134680
F	−2.815951	−3.799115	1.100731
F	−4.151251	−2.344034	0.040828
F	2.379921	−4.133002	−0.216046
F	3.664741	−2.956028	1.192944
F	3.896755	−2.688828	−1.014984

$\mathbf{1}_{\mathbf{Rh}}$

E= -2957.4048672au

Rh	−2.367286	−0.021996	1.138282
O	−1.165469	−0.309895	2.808577
C	0.102110	−0.370654	2.650847
C	0.949282	−0.505226	3.915630
Rh	−0.296701	−0.018295	−0.213342
O	−2.139989	2.031615	1.347091
O	−3.402201	0.267895	−0.639388
O	−2.453859	−2.069361	0.844516
O	0.756549	−0.273779	1.547763
O	−1.480155	0.222159	−1.899840
O	−0.511544	−2.073443	−0.385362
O	−0.257232	2.041000	0.031281
C	−1.165498	2.601803	0.749481
C	−2.754230	0.313194	−1.739668
C	−1.526794	−2.635560	0.168657
C	−1.091568	4.126329	0.825169
C	−3.572885	0.419307	−3.025604
C	−1.582011	−4.157027	0.033796
N	1.471504	−0.015441	−1.365933
C	1.922702	0.023874	−2.540310
C	2.993296	0.044143	−1.491530
C	3.723216	−1.231836	−1.170119
C	4.401542	−1.939296	−2.174335
H	4.400210	−1.562521	−3.194863
F	2.152187	−1.129587	3.647380
F	1.224991	0.755762	4.424177
F	0.294034	−1.228396	4.886015
F	0.220057	4.562116	0.815976
F	−1.728562	4.670848	−0.282428
F	−1.702162	4.611204	1.957126
F	−3.836108	−0.855506	−3.508676
F	−4.771914	1.058052	−2.814688
F	−2.877071	1.107462	−4.000861
F	−1.262109	−4.548121	−1.251863
F	−0.661116	−4.731073	0.898893
F	−2.827719	−4.651723	0.339988
C	3.738452	−1.718558	0.149388
H	3.208382	−1.182280	0.929746
C	5.084971	−3.122619	−1.868296
H	5.607191	−3.663461	−2.651477
C	5.090608	−3.605959	−0.555497
H	5.616239	−4.524976	−0.316882
C	4.415312	−2.903425	0.450698
H	4.413802	−3.277873	1.469080
C	3.645621	1.355245	−1.139527
C	5.043950	1.431494	−0.995313
C	2.879351	2.523386	−0.964334
C	5.659390	2.649139	−0.690854
H	5.647445	0.539273	−1.115836
C	3.498016	3.735248	−0.645408
H	1.799615	2.485888	−1.037403
C	4.889803	3.804789	−0.513538
H	6.738620	2.691916	−0.584664
H	2.886396	4.617664	−0.488399
H	5.368516	4.747107	−0.267592
C	1.482415	0.079207	−3.946873
H	0.394979	0.174741	−4.003853
H	1.953716	0.926729	−4.456921
H	1.792096	−0.831871	−4.472930

$\mathbf{TS}_{\mathbf{(1\text{-}2)Rh}}$

E= -2957.3784446au

Rh	−1.841187	−0.091161	−1.566215
O	−0.162303	−0.612610	−2.666389
C	0.951601	−0.733030	−2.052799

C	2.167155	-1.165875	-2.872261
Rh	-0.407465	-0.056532	0.453385
O	-2.186154	-2.098865	-1.185380
O	-3.433622	0.420387	-0.354867
O	-1.395520	1.918981	-1.815615
O	1.179678	-0.550531	-0.800751
O	-2.119219	0.437133	1.531242
O	-0.090086	1.959314	0.078054
O	-0.826453	-2.080772	0.669096
C	-1.611947	-2.642147	-0.179279
C	-3.229830	0.568901	0.900974
C	-0.637052	2.489248	-0.956002
C	-1.918573	-4.114205	0.093350
C	-4.419496	1.012308	1.751702
C	-0.279961	3.950922	-1.224276
N	0.647883	-0.091091	2.297120
C	1.652987	0.027677	3.044364
C	2.679398	0.177657	2.002143
C	2.942827	1.501713	1.443479
C	2.704385	2.655104	2.229981
H	2.329124	2.547420	3.243138
F	3.211758	-0.262771	-2.703751
F	2.612040	-2.405641	-2.444563
F	1.887683	-1.243601	-4.214047
F	-0.770525	-4.793805	0.459395
F	-2.826128	-4.216636	1.137254
F	-2.455479	-4.738575	-1.008034
F	-4.327183	2.376339	1.995878
F	-5.617604	0.769445	1.120273
F	-4.430588	0.361548	2.968897
F	-0.035038	4.637574	-0.053243
F	0.873815	4.007804	-2.000259
F	-1.283657	4.601993	-1.905347
C	3.412314	1.674665	0.118484
H	3.546454	0.811297	-0.518379
C	2.947274	3.928332	1.720777
H	2.760898	4.801677	2.336777
C	3.419114	4.079980	0.409736
H	3.594173	5.072453	0.007952
C	3.646505	2.951405	-0.388603
H	3.986388	3.068703	-1.411718
C	3.368533	-1.042747	1.549340
C	4.717901	-0.972780	1.124949
C	2.750848	-2.314119	1.619319
C	5.416560	-2.132057	0.783673
H	5.223468	-0.015375	1.095432
C	3.450530	-3.463333	1.255336
H	1.709487	-2.391247	1.908154
C	4.786269	-3.380087	0.839501
H	6.453198	-2.058408	0.471937
H	2.949421	-4.424889	1.289207
H	5.327792	-4.277905	0.560776
C	1.764552	-0.117917	4.531698
H	0.774638	-0.283504	4.964451
H	2.413341	-0.967387	4.778537
H	2.212019	0.775943	4.982537

$\mathbf{2}_{\mathbf{Rh}}$

E= -2957.37912au

Rh	-2.866803	-0.122528	0.271439
O	-2.669359	1.805692	1.045255
C	-1.512333	2.340134	1.088543
C	-1.410756	3.725955	1.726182
Rh	-0.369636	-0.089019	-0.108332
O	-3.063533	0.671415	-1.637660
O	-2.836259	-2.043444	-0.539462
O	-2.457069	-0.919648	2.159695
O	-0.390643	1.834007	0.710323
O	-0.555402	-2.011536	-0.859173
O	-0.180730	-0.841467	1.822241
O	-0.787537	0.681323	-1.999345
C	-2.012327	0.888783	-2.331186
C	-1.725760	-2.549605	-0.906319
C	-1.244853	-1.094794	2.505382
C	-2.206941	1.527387	-3.706609
C	-1.751125	-3.948740	-1.520842
C	-0.967500	-1.648413	3.902422
N	1.585448	0.157371	-0.458410

C	2.559217	-0.610198	-0.068510
C	3.900202	-0.013906	-0.178772
C	3.988245	1.421039	-0.203587
C	2.953234	2.229135	0.359158
H	2.210391	1.786471	1.008270
F	-1.051334	3.601305	3.062329
F	-0.437061	4.495588	1.104423
F	-2.598753	4.413509	1.662422
F	-1.919463	2.885237	-3.634161
F	-1.360686	0.965413	-4.643158
F	-3.499343	1.389508	-4.159867
F	-0.727121	-4.727589	-1.005795
F	-2.941082	-4.595818	-1.286038
F	-1.566320	-3.864861	-2.893730
F	-0.095301	-2.725430	3.827346
F	-0.365473	-0.675992	4.688324
F	-2.112506	-2.066007	4.535610
C	5.045310	2.073537	-0.912038
H	5.819864	1.476197	-1.376892
C	2.948790	3.612292	0.167252
H	2.142248	4.201859	0.587564
C	3.977971	4.218835	-0.556157
H	3.974781	5.294148	-0.702877
C	5.030748	3.447273	-1.089697
H	5.816987	3.927349	-1.661673
C	5.107144	-0.837841	-0.244956
C	6.287847	-0.451906	0.437172
C	5.123308	-2.031606	-1.008913
C	7.438573	-1.236397	0.362339
H	6.279210	0.443052	1.048710
C	6.284661	-2.795397	-1.101591
H	4.232366	-2.332460	-1.548187
C	7.441567	-2.404656	-0.411029
H	8.328814	-0.941913	0.907203
H	6.290613	-3.695482	-1.706309
H	8.338895	-3.011368	-0.472505
C	2.375291	-2.013110	0.506201
H	1.711295	-1.953268	1.372156
H	1.888936	-2.664881	-0.225329
H	3.318341	-2.462981	0.817918

$TS_{(2\text{-}3)Rh}$

E= -2957.3786382au

C	2.616397	-0.520281	-0.159242
N	1.611921	0.251553	-0.453679
O	-0.094861	-0.965617	1.765513
C	3.936237	0.130281	-0.181215
C	3.885502	1.548161	-0.140706
C	2.669109	2.178808	0.297707
H	2.064393	1.718171	1.068588
C	4.889773	2.361261	-0.764106
H	5.805310	1.897211	-1.109841
C	2.419236	3.530441	-0.016020
H	1.488704	3.983196	0.304277
C	3.390072	4.271565	-0.672826
H	3.213029	5.319860	-0.891292
C	4.635949	3.689772	-1.031799
H	5.376808	4.289380	-1.549146
O	-0.469236	1.778924	0.868106
O	-0.827908	0.826857	-1.910197
O	-0.451957	-1.930862	-1.001295
Rh	-0.355112	-0.071208	-0.090103
Rh	-2.834738	-0.276889	0.296783
C	-1.555254	-3.880723	-1.797082
C	-1.585364	-2.538703	-1.066223
O	-2.715855	-2.132463	-0.638693
C	-2.308058	1.688559	-3.555953
C	-2.065234	0.970888	-2.228072
O	-3.094872	0.627953	-1.552526
C	-1.581496	3.554958	1.977563
C	-1.616950	2.195751	1.279347
O	-2.740484	1.600372	1.198404
C	-0.814856	-1.949294	3.796055
C	-1.134542	-1.317342	2.441944
O	-2.359082	-1.171265	2.124619
F	-1.918653	-2.527639	4.374079
F	0.162069	-2.923203	3.655955
F	-0.324355	-0.983084	4.663522

F	-3.604494	1.540448	-3.992343
F	-1.464003	1.210576	-4.540218
F	-2.057606	3.046928	-3.403461
F	-2.836374	4.070797	2.182783
F	-0.857936	4.472335	1.222938
F	-0.949223	3.439204	3.207296
F	-2.598652	-4.693448	-1.417514
F	-0.371925	-4.553812	-1.547831
F	-1.644150	-3.671818	-3.166278
C	2.465170	-1.981960	0.245281
H	1.892348	-2.033466	1.176058
H	1.900806	-2.532509	-0.511435
H	3.430408	-2.463972	0.400614
C	5.199653	-0.611380	-0.248268
C	6.304023	-0.216401	0.543286
C	5.350360	-1.715908	-1.120027
C	7.513942	-0.907733	0.470086
H	6.192346	0.614065	1.231827
C	6.567625	-2.391405	-1.202555
H	4.520375	-2.018014	-1.749153
C	7.649454	-1.993611	-0.404567
H	8.346808	-0.605522	1.095807
H	6.674638	-3.226541	-1.886209
H	8.591125	-2.529363	-0.462388

$TS_{(2\text{-}4)Rh}$

E= -2957.3355036au

C	2.604304	-0.558774	-0.730068
N	1.513790	0.167913	-0.916233
O	0.181603	-0.762332	1.688046
C	3.907118	0.047953	-0.701513
C	3.950255	1.484206	-0.579917
C	2.752806	2.212872	-0.493533
H	1.730297	1.255857	-0.961164
C	5.143226	2.267526	-0.679241
H	6.089648	1.768004	-0.856693
C	2.626589	3.572645	-0.672214
H	1.661138	4.067118	-0.660188
C	3.826738	4.315430	-0.654389
H	3.784769	5.397721	-0.575542
C	5.068384	3.655196	-0.677364
H	5.981175	4.238802	-0.735038
O	-0.387989	1.879318	0.499658
O	-1.216845	0.607404	-1.966746
O	-0.686182	-2.039977	-0.814134
Rh	-0.432116	-0.080382	-0.170288
Rh	-2.774245	-0.199542	0.678316
C	-1.902062	-4.054498	-1.146109
C	-1.805910	-2.633478	-0.591749
O	-2.837370	-2.157208	-0.008884
C	-2.977978	1.277512	-3.417074
C	-2.493215	0.722319	-2.077832
O	-3.379600	0.470201	-1.191082
C	-1.302297	3.821922	1.512475
C	-1.439676	2.370025	1.055595
O	-2.544075	1.775277	1.291657
C	-0.153964	-1.463583	3.931294
C	-0.710850	-1.001296	2.585377
O	-1.975567	-0.864668	2.480843
F	-1.133967	-1.980672	4.744152
F	0.814983	-2.435422	3.746670
F	0.437305	-0.393812	4.587241
F	-4.330124	1.095839	-3.588699
F	-2.321447	0.671887	-4.470672
F	-2.712772	2.639792	-3.474887
F	-2.520917	4.395266	1.782109
F	-0.675328	4.582946	0.534989
F	-0.525372	3.885815	2.658799
F	-2.933984	-4.760361	-0.574451
F	-0.725333	-4.747378	-0.922242
F	-2.113375	-4.006760	-2.516498
C	5.143119	-0.758365	-0.690590
C	6.114129	-0.582487	0.321711
C	5.388071	-1.717833	-1.699115
C	7.282433	-1.348117	0.328265
H	5.931000	0.133483	1.115653
C	6.562559	-2.471964	-1.695642
H	4.659834	-1.851133	-2.492617

C	7.511557	-2.291955	-0.680441
H	8.009328	-1.213175	1.122387
H	6.739064	-3.197388	-2.482797
H	8.420797	-2.883962	-0.674992
C	2.413206	-2.021473	-0.361075
H	3.349711	-2.571990	-0.431740
H	2.049237	-2.083310	0.670883
H	1.663650	-2.489904	-1.000344

$\mathbf{3}_{\mathbf{Rh}}$

E= -2957.4292872au

Rh	2.746717	-0.544185	0.331285
O	3.196720	0.871653	-1.117848
C	2.238292	1.489485	-1.690879
C	2.586055	2.534647	-2.749645
Rh	0.346785	-0.033922	-0.063028
O	2.721552	0.953016	1.771255
O	2.132613	-1.920687	1.757847
O	2.590369	-2.000746	-1.137536
O	0.975922	1.331227	-1.492686
O	-0.086204	-1.431089	1.408332
O	0.367211	-1.534491	-1.494769
O	0.505974	1.434471	1.394402
C	1.639873	1.596533	1.983973
C	0.882367	-2.060628	1.976308
C	1.460783	-2.177743	-1.708105
C	1.697717	2.737949	2.998492
C	0.452856	-3.048013	3.060455
C	1.386517	-3.233950	-2.810339
N	-1.703341	0.466963	-0.331657
C	-2.750722	-0.333865	-0.355546
C	-4.009054	0.412412	-0.240499
C	-3.671157	1.741414	-0.126882
C	-2.173876	1.833098	-0.081035
H	-1.885822	2.002913	0.979238
F	1.917941	3.720397	-2.477744
F	2.183502	2.097851	-4.000381
F	3.932729	2.798530	-2.793096
F	2.684035	2.536293	3.935034
F	0.493138	2.880206	3.657705
F	1.964680	3.928017	2.333342
F	1.465626	-3.910730	3.402672
F	0.066543	-2.353307	4.197234
F	-0.630567	-3.795422	2.630730
F	0.177064	-3.903411	-2.764451
F	1.489489	-2.622088	-4.050640
F	2.396891	-4.159795	-2.698887
C	-1.607440	3.030488	-0.796895
C	-4.441503	2.954793	-0.190385
H	-5.515939	2.923626	-0.050922
C	-2.397459	4.123601	-0.929364
C	-3.807808	4.106622	-0.563914
H	-4.376142	5.025065	-0.670474
H	-0.565185	3.027495	-1.088202
H	-1.989276	5.038108	-1.347237
C	-5.373919	-0.159648	-0.259106
C	-6.276932	0.138635	0.781072
C	-5.811060	-0.978536	-1.319692
C	-7.579158	-0.368894	0.761571
H	-5.945638	0.754837	1.611009
C	-7.113197	-1.486361	-1.335424
H	-5.137015	-1.195739	-2.142247
C	-8.000549	-1.183942	-0.295544
H	-8.260684	-0.133977	1.572854
H	-7.436596	-2.110824	-2.161934
H	-9.010851	-1.579557	-0.309277
C	-2.640746	-1.826860	-0.424995
H	-2.192571	-2.211674	0.497456
H	-3.621714	-2.285501	-0.549550
H	-1.988950	-2.131802	-1.248007

$\mathbf{TS}_{\mathbf{(3\text{-}4)Rh}}$

E= -2957.3920309au

Rh	-2.748355	-0.550193	0.285707
O	-2.728609	0.838498	1.822751
C	-1.638755	1.451645	2.085887
C	-1.654279	2.489847	3.207071
Rh	-0.356860	-0.030429	-0.077468

O	-3.179116	0.965979	-1.070156
O	-2.611217	-1.903511	-1.280290
O	-2.149516	-2.019175	1.617060
O	-0.505884	1.317571	1.490331
O	-0.392810	-1.412948	-1.624448
O	0.072008	-1.534097	1.282953
O	-0.956260	1.437868	-1.408636
C	-2.218414	1.616028	-1.601194
C	-1.489385	-2.035775	-1.878338
C	-0.897547	-2.191992	1.812302
C	-2.558621	2.756124	-2.559578
C	-1.426892	-2.997437	-3.064425
C	-0.482228	-3.260090	2.823251
N	1.718283	0.474123	-0.402852
C	2.821480	-0.358898	-0.383770
C	4.014145	0.378922	-0.305817
C	3.675820	1.759621	-0.318161
C	2.241528	1.849000	-0.387394
H	1.810101	1.323469	-1.453472
F	-1.415666	3.749036	2.673989
F	-0.660340	2.221372	4.129276
F	-2.860461	2.519951	3.863264
F	-3.911052	2.880117	-2.757020
F	-1.951973	2.550333	-3.785756
F	-2.079685	3.951640	-2.041565
F	-2.481135	-3.878995	-3.065148
F	-1.459543	-2.275071	-4.248268
F	-0.250356	-3.723584	-3.040051
F	0.660293	-3.913915	2.399033
F	-0.206016	-2.663366	4.044107
F	-1.471177	-4.196200	3.011721
C	1.557992	3.090697	-0.170316
C	4.431959	2.954458	-0.204543
H	5.514099	2.911567	-0.167206
C	2.338124	4.222524	-0.065379
C	3.763341	4.158722	-0.089649
H	4.328684	5.079037	0.011955
H	0.478837	3.135300	-0.145505
H	1.857394	5.187464	0.053747
C	5.388242	-0.171756	-0.282289
C	6.368898	0.319732	-1.167724
C	5.748888	-1.181808	0.631149
C	7.671163	-0.186693	-1.140836
H	6.101089	1.084837	-1.889464
C	7.051939	-1.687370	0.655218
H	5.010625	-1.552689	1.334460
C	8.016832	-1.191666	-0.229565
H	8.412756	0.198189	-1.833600
H	7.314775	-2.461905	1.368482
H	9.028308	-1.584123	-0.208837
C	2.669653	-1.841799	-0.552512
H	1.983568	-2.071365	-1.373417
H	3.638194	-2.298253	-0.766897
H	2.260186	-2.307924	0.349875

$\mathbf{4}_{\mathbf{Rh}}$

E= -2957.4696673au

Rh	-2.161907	-0.593719	1.327047
O	-0.793220	-1.882637	2.202742
C	0.381589	-1.957534	1.703596
C	1.380273	-2.854726	2.433251
Rh	-0.416759	-0.008501	-0.323445
O	-1.458119	0.946376	2.511336
O	-3.408684	0.739522	0.331213
O	-2.750207	-2.095888	0.011164
O	0.836039	-1.322727	0.682702
O	-1.791761	1.254707	-1.217289
O	-1.124907	-1.543773	-1.518288
O	0.169708	1.492736	0.982391
C	-0.468821	1.641108	2.087659
C	-2.965413	1.353716	-0.696255
C	-2.122045	-2.240230	-1.090899
C	-0.027736	2.824757	2.947651
C	-3.919888	2.280938	-1.446903
C	-2.550802	-3.379309	-2.015048
N	1.095928	0.504216	-1.938968
C	2.270638	-0.337522	-1.848061
C	3.341805	0.423456	-1.470864

C	2.911453	1.827282	−1.434960
C	1.548373	1.858656	−1.787099
F	1.989599	−2.140188	3.452804
F	2.369339	−3.300567	1.573867
F	0.762176	−3.954275	2.983394
F	−0.458225	2.698542	4.248007
F	−0.565059	3.993464	2.423720
F	1.346061	2.950019	2.953087
F	−4.336456	1.663665	−2.618347
F	−5.029588	2.593088	−0.701793
F	−3.278423	3.457689	−1.792334
F	−3.720863	−3.965907	−1.601263
F	−2.725870	−2.914350	−3.306530
F	−1.559925	−4.350255	−2.042276
C	0.819135	3.038400	−1.896991
C	3.569552	3.028487	−1.143026
H	4.610020	3.031513	−0.839700
C	1.503405	4.234505	−1.632791
C	2.854846	4.227653	−1.251716
H	3.352450	5.166941	−1.034821
H	−0.235491	3.037901	−2.147192
H	0.973078	5.177377	−1.711656
C	4.696706	−0.071824	−1.155161
C	5.838103	0.556920	−1.693810
C	4.872855	−1.175160	−0.294973
C	7.118426	0.089329	−1.386949
H	5.717085	1.397865	−2.368767
C	6.155861	−1.638465	0.010170
H	4.004993	−1.647074	0.153185
C	7.281627	−1.009314	−0.534045
H	7.987337	0.578960	−1.815090
H	6.275502	−2.484090	0.679832
H	8.276825	−1.368896	−0.293174
C	2.163331	−1.790224	−2.182517
H	1.588534	−1.944173	−3.104569
H	3.160571	−2.211780	−2.327724
H	1.667928	−2.359449	−1.389777
H	0.504307	0.325037	−2.750165

H_2O

E= -76.4178778au

O	0.000000	0.000000	0.118537
H	0.000000	0.759405	−0.474150
H	0.000000	−0.759405	−0.474150

$3'_{Fe}$

E= -1096.3906144au

N	−0.089391	−0.136040	0.208949
C	−1.225164	−0.815225	0.106755
C	−2.375648	0.050370	−0.113703
C	−1.891114	1.344510	−0.122241
C	−0.439180	1.278159	0.213687
H	−0.395960	1.512983	1.325508
C	0.412508	2.348739	−0.381505
C	−2.469631	2.611922	−0.465650
H	−3.543920	2.706786	−0.578026
C	−0.187292	3.507640	−0.761860
C	−1.633011	3.654978	−0.761330
H	−2.050616	4.609751	−1.065635
H	1.490501	2.225050	−0.377951
H	0.412630	4.347706	−1.097992
C	−3.783605	−0.373617	−0.288919
C	−4.793840	0.175973	0.525944
C	−4.151500	−1.304138	−1.281757
C	−6.130563	−0.195739	0.354348
H	−4.520127	0.879366	1.305962
C	−5.488134	−1.677362	−1.448833
H	−3.390635	−1.715699	−1.937422
C	−6.481852	−1.125046	−0.631658
H	−6.894862	0.233020	0.994852
H	−5.754203	−2.392644	−2.220679
H	−7.519104	−1.416266	−0.762296
C	−1.278272	−2.301217	0.303067
H	−1.297828	−2.531220	1.377305
H	−2.177619	−2.733552	−0.137910
H	−0.394547	−2.788737	−0.118610
Cl	2.323100	−2.891851	−0.417387
Fe	1.822208	−0.918700	0.601804

Cl	2.396420	−0.264956	2.748320
H	6.251376	0.712889	−1.503530
C	5.183443	0.948530	−1.491883
C	4.488474	0.413194	−0.240722
C	4.406641	0.245750	−2.628093
H	5.071811	2.037101	−1.560027
H	4.525316	1.066611	0.631191
H	4.846597	−0.585062	0.032579
C	2.960689	0.220514	−2.110860
H	4.490687	0.767981	−3.585360
H	4.777344	−0.776024	−2.762901
H	2.430975	−0.702393	−2.354122
H	2.376172	1.087167	−2.434630
H	0.203181	2.350120	3.511057
O	−0.213211	1.530567	3.219967
H	0.513439	0.878719	3.246371
O	3.066731	0.304797	−0.633951

TS'$_{(3\text{-}5)Fe}$

E= -1096.3843349au

N	−0.087682	−0.146910	0.059089
C	−1.257543	−0.837589	−0.006940
C	−2.375723	0.018596	−0.192435
C	−1.864167	1.334082	−0.226247
C	−0.427648	1.227288	0.008881
H	−0.427646	1.426739	1.330982
C	0.429682	2.351683	−0.313610
C	−2.427709	2.615463	−0.480944
H	−3.498744	2.721263	−0.614883
C	−0.162302	3.570455	−0.556896
C	−1.587602	3.701639	−0.627688
H	−2.009447	4.679408	−0.839064
H	1.508221	2.232390	−0.277580
H	0.454359	4.447389	−0.726471
C	−3.798410	−0.370929	−0.306835
C	−4.781543	0.273338	0.472764
C	−4.213525	−1.372930	−1.207978
C	−6.130474	−0.074078	0.357061
H	−4.477529	1.033500	1.185569
C	−5.562037	−1.725178	−1.316718
H	−3.476039	−1.858695	−1.838760
C	−6.526267	−1.076919	−0.535982
H	−6.870638	0.430699	0.970447
H	−5.860439	−2.498656	−2.017672
H	−7.573242	−1.349424	−0.622871
C	−1.277231	−2.324960	0.201261
H	−0.879764	−2.582130	1.191710
H	−2.292931	−2.718658	0.136921
H	−0.650124	−2.841775	−0.533424
Fe	1.756413	−0.958756	0.491882
Cl	2.439716	−2.926897	−0.391901
Cl	2.135188	−0.260469	2.739413
O	3.142554	0.291547	−0.532620
C	4.518265	0.378036	−0.000254
C	3.183058	0.266184	−2.015119
C	5.314877	1.015310	−1.137408
H	4.461169	0.960498	0.919379
H	4.865168	−0.635939	0.226461
C	4.670040	0.378612	−2.390083
H	2.725163	−0.668017	−2.346765
H	2.588590	1.117989	−2.357936
H	6.385180	0.803169	−1.062258
H	5.180210	2.103334	−1.140354
H	4.820533	0.976365	−3.293440
H	5.092234	−0.616480	−2.566409
H	−0.076524	2.306003	2.968104
O	−0.341660	1.428787	2.659194
H	0.436327	0.820979	2.836484

5'$_{Fe}$

E= -1096.3973473au

N	−0.092080	−0.166013	−0.007232
C	−1.295574	−0.873134	−0.057649
C	−2.379641	−0.017859	−0.236046
C	−1.834453	1.319804	−0.300587
C	−0.414040	1.176375	−0.172029
H	−0.582054	1.334721	1.902819
C	0.434149	2.305055	−0.207215

C	−2.387471	2.604808	−0.485027
H	−3.457895	2.726750	−0.612962
C	−0.144501	3.565608	−0.371926
C	−1.543350	3.713109	−0.514183
H	−1.962560	4.704318	−0.656315
H	1.511405	2.189713	−0.126386
H	0.491177	4.445538	−0.407511
C	−3.808222	−0.380800	−0.334427
C	−4.785367	0.340138	0.385855
C	−4.243067	−1.442724	−1.155439
C	−6.139757	0.009270	0.292354
H	−4.472662	1.150098	1.037027
C	−5.597405	−1.778727	−1.241442
H	−3.513899	−1.988235	−1.745232
C	−6.552820	−1.053968	−0.519647
H	−6.872163	0.575737	0.859881
H	−5.907449	−2.599442	−1.881364
H	−7.604689	−1.312327	−0.590491
C	−1.294164	−2.362020	0.131436
H	−0.666073	−2.655947	0.982616
H	−2.304799	−2.732008	0.319415
H	−0.899595	−2.889396	−0.747006
Fe	1.684580	−0.978895	0.344236
Cl	2.638715	−2.975765	−0.006036
Cl	2.115196	−0.099886	2.737790
O	3.107217	0.259397	−0.620147
C	4.490955	0.360006	−0.112181
C	3.111832	0.298988	−2.102220
C	5.258254	1.029785	−1.251524
H	4.444476	0.933273	0.814458
H	4.853606	−0.652439	0.094292
C	4.589017	0.423749	−2.506482
H	2.641199	−0.617275	−2.466231
H	2.509745	1.164230	−2.392185
H	6.330708	0.820574	−1.205786
H	5.119134	2.116657	−1.223724
H	4.718123	1.046439	−3.396027
H	5.010968	−0.564373	−2.718917
H	−0.033464	2.335127	2.953462
O	−0.229898	1.396915	2.819075
H	0.870936	0.692394	2.825672

4'$_{Fe}$

E= -1096.441276au

C	0.214378	0.931059	−1.607626
N	−0.126470	−0.438292	−1.421969
C	1.510676	1.140644	−1.087787
C	2.019386	−0.159608	−0.653701
C	1.047679	−1.094232	−0.905565
C	−0.547736	1.960358	−2.163215
H	−1.552543	1.785754	−2.531291
C	2.065024	2.431653	−1.120317
H	3.063923	2.613348	−0.739452
C	0.025135	3.237159	−2.192158
C	1.314216	3.470026	−1.675705
H	1.731617	4.471021	−1.715681
H	−0.538023	4.060896	−2.618099
C	3.356428	−0.397842	−0.062049
C	4.207018	−1.407410	−0.554734
C	3.815208	0.401473	1.005207
C	5.467048	−1.621457	0.012408
H	3.885601	−2.008208	−1.398836
C	5.076176	0.188685	1.569044
H	3.172741	1.182341	1.399833
C	5.906047	−0.825504	1.076512
H	6.108581	−2.402758	−0.382946
H	5.409174	0.810748	2.394063
H	6.885359	−0.990437	1.514105
C	1.034965	−2.576903	−0.706772
H	1.031332	−3.113638	−1.666291
H	1.921981	−2.892550	−0.153468
H	0.149028	−2.899883	−0.147898
Cl	−3.787628	0.571899	−1.161745
Fe	−2.096388	−0.698742	−0.190467
Cl	−2.315141	−2.725434	0.903979
H	−3.687168	1.104995	1.828614
C	−2.841722	0.751667	2.420984
C	−2.290128	1.771576	3.420638

O	-1.728336	0.513946	1.478267
H	-3.087677	-0.207823	2.886711
C	-0.783938	1.428043	3.465812
H	-2.770763	1.689170	4.399521
H	-2.439823	2.792527	3.051253
C	-0.471261	1.068012	2.009005
H	-0.170344	2.259528	3.824450
H	-0.608926	0.566895	4.120612
H	0.302552	0.305954	1.895495
H	-0.212920	1.944576	1.406977
O	-2.470996	-2.031513	-2.158570
H	-2.712006	-2.800169	-1.616695
H	-3.298987	-1.551934	-2.329556
H	-0.597180	-0.918763	-2.190923

3'$_{Rh}$

E= -3033.8628392au

Rh	-2.800124	0.517703	0.327258
O	-3.212740	-0.492788	-1.433973
C	-2.242161	-0.968706	-2.114226
C	-2.568659	-1.726921	-3.400249
Rh	-0.387327	0.047904	-0.101968
O	-2.866841	-1.277943	1.377700
O	-2.191483	1.494019	2.064909
O	-2.565631	2.272764	-0.744892
O	-0.985114	-0.888804	-1.848193
O	0.021638	0.975841	1.714987
O	-0.337860	1.851461	-1.123232
O	-0.649382	-1.721511	0.957869
C	-1.804219	-1.974100	1.471379
C	-0.956949	1.503594	2.374249
C	-1.414154	2.546980	-1.226830
C	-1.855289	-3.267951	2.282294
C	-0.532514	2.206397	3.662529
C	-1.296359	3.811536	-2.077069
N	1.657777	-0.375792	-0.449718
C	2.701672	0.434442	-0.367124
C	3.961805	-0.299130	-0.432133
C	3.636378	-1.636501	-0.530373
C	2.150573	-1.752109	-0.410155
H	1.979776	-1.997844	0.672191
F	-1.992205	-2.987997	-3.358089
F	-2.051029	-1.057225	-4.494851
F	-3.921680	-1.877131	-3.581284
F	-3.046739	-3.428627	2.939085
F	-0.833792	-3.257292	3.233499
F	-1.649761	-4.360834	1.460205
F	0.325205	3.253740	3.365705
F	-1.602058	2.701943	4.363038
F	0.151927	1.313370	4.474754
F	-2.249079	4.743137	-1.736818
F	-0.050120	4.390666	-1.929598
F	-1.462037	3.485891	-3.415182
C	1.533336	-2.875868	-1.179393
C	4.404940	-2.816575	-0.805385
H	5.486930	-2.783791	-0.750113
C	2.316621	-3.939504	-1.491895
C	3.751039	-3.931775	-1.254306
H	4.317857	-4.820843	-1.511935
H	0.470406	-2.863465	-1.383117
H	1.880180	-4.814614	-1.962129
C	5.320916	0.284671	-0.390135
C	6.263001	-0.192902	0.543580
C	5.712963	1.299642	-1.286027
C	7.559052	0.329341	0.578629
H	5.965319	-0.958954	1.252568
C	7.008835	1.822310	-1.246309
H	5.007543	1.661158	-2.027591
C	7.935627	1.339116	-0.314774
H	8.270568	-0.045604	1.307453
H	7.296490	2.600029	-1.946511
H	8.941169	1.746055	-0.285237
C	2.584900	1.915138	-0.157623
H	2.024111	2.125019	0.758807
H	3.571728	2.370605	-0.071304
H	2.041840	2.389199	-0.979598
H	1.113389	-2.031862	2.888203
O	1.843356	-1.434397	2.684353

H	1.420177	-0.569510	2.595932

TS'$_{(3\text{-}5)Rh}$

E= -3033.8491523au

Rh	2.786153	-0.614011	0.279098
O	3.224229	0.613518	-1.332237
C	2.263698	1.203435	-1.932925
C	2.604347	2.127364	-3.101733
Rh	0.371281	-0.057997	-0.088209
O	2.877205	1.047305	1.541503
O	2.169402	-1.802796	1.872370
O	2.518410	-2.207478	-1.006316
O	1.006798	1.123690	-1.667837
O	-0.041865	-1.243257	1.570412
O	0.307589	-1.679017	-1.356508
O	0.646127	1.527297	1.290208
C	1.834470	1.723868	1.778332
C	0.928595	-1.851465	2.161998
C	1.366437	-2.388502	-1.530154
C	1.966970	2.942979	2.690859
C	0.501598	-2.692383	3.364325
C	1.217755	-3.542426	-2.521464
N	-1.659755	0.408532	-0.455207
C	-2.739970	-0.423796	-0.340072
C	-3.953301	0.302273	-0.410770
C	-3.602274	1.665288	-0.584272
C	-2.149791	1.727517	-0.557561
H	-2.078453	2.031890	0.815291
F	2.083601	3.391138	-2.860077
F	2.042713	1.650003	-4.271683
F	3.960038	2.247657	-3.286183
F	3.046143	2.845161	3.529379
F	0.819110	3.078680	3.463671
F	2.099601	4.088484	1.924479
F	-0.508028	-3.567988	3.003728
F	1.541815	-3.416634	3.888382
F	0.004187	-1.857301	4.357947
F	2.177255	-4.507578	-2.322455
F	-0.025064	-4.134449	-2.402514
F	1.343679	-3.061681	-3.815707
C	-1.478803	2.928929	-0.989529
C	-4.341867	2.856738	-0.810352
H	-5.425884	2.828609	-0.809355
C	-2.240341	4.061581	-1.192292
C	-3.663648	4.027533	-1.092818
H	-4.222518	4.939313	-1.277900
H	-0.404459	2.940969	-1.119860
H	-1.752675	4.991205	-1.465726
C	-5.332204	-0.228544	-0.314515
C	-6.257561	0.358022	0.574546
C	-5.769084	-1.303903	-1.114873
C	-7.569119	-0.116518	0.664298
H	-5.937685	1.182115	1.205159
C	-7.078802	-1.783794	-1.017713
H	-5.083734	-1.746271	-1.830336
C	-7.984277	-1.192750	-0.128836
H	-8.263624	0.348369	1.357444
H	-7.395109	-2.611652	-1.644671
H	-9.001640	-1.563765	-0.057314
C	-2.603671	-1.904468	-0.129041
H	-1.993815	-2.131617	0.749426
H	-3.586693	-2.357607	0.009476
H	-2.119693	-2.380014	-0.988538
H	-0.840203	2.009957	2.010302
O	-1.828021	2.098389	2.028970
H	-2.179437	1.296591	2.445184

5'$_{Rh}$

E= -3033.8614617au

Rh	2.626091	-0.406762	0.904761
O	3.452502	0.908845	-0.452726
C	2.705423	1.399231	-1.365341
C	3.329413	2.374372	-2.362903
Rh	0.427563	-0.047615	-0.256933
O	2.097925	1.210934	2.131024
O	1.619402	-1.721129	2.183839
O	2.954546	-1.957542	-0.420929
O	1.451670	1.177126	-1.554487

O	-0.433928	-1.252364	1.271801
O	0.916384	-1.664761	-1.448568
O	0.042642	1.477969	1.136008
C	0.963695	1.765984	2.003633
C	0.363840	-1.843102	2.116732
C	2.052883	-2.243154	-1.282794
C	0.613034	2.925361	2.935815
C	-0.336128	-2.792749	3.087325
C	2.377729	-3.361999	-2.272928
N	-1.414398	0.331111	-1.252497
C	-2.486705	-0.528348	-1.119917
C	-3.691321	0.195281	-0.956257
C	-3.332099	1.603599	-1.089268
C	-1.917193	1.635444	-1.251891
H	-3.001319	0.257171	0.694069
F	2.643638	3.579849	-2.323867
F	3.238491	1.870902	-3.647189
F	4.651374	2.619781	-2.082707
F	1.409324	2.948203	4.052603
F	-0.710946	2.807067	3.344071
F	0.748518	4.128739	2.268836
F	-0.732700	-3.937601	2.418369
F	0.468347	-3.148305	4.136543
F	-1.476692	-2.176575	3.591330
F	3.263399	-4.268547	-1.734554
F	1.237124	-4.041564	-2.647686
F	2.951126	-2.816953	-3.411717
C	-1.240275	2.859232	-1.412583
C	-4.077678	2.796576	-1.110234
H	-5.159359	2.771780	-1.029003
C	-1.996454	4.031336	-1.413686
C	-3.400471	4.003887	-1.266725
H	-3.958130	4.934465	-1.293390
H	-0.169330	2.889278	-1.565923
H	-1.495598	4.984646	-1.548831
C	-5.077258	-0.338531	-0.950481
C	-6.018162	0.139778	-0.014214
C	-5.500833	-1.304819	-1.885246
C	-7.331045	-0.339059	-0.005817
H	-5.713573	0.884379	0.715549
C	-6.812853	-1.788225	-1.871283
H	-4.804658	-1.658970	-2.637871
C	-7.732818	-1.309023	-0.931790
H	-8.037495	0.040492	0.725836
H	-7.118509	-2.531098	-2.601411
H	-8.751476	-1.683010	-0.924184
C	-2.326010	-2.020215	-1.179686
H	-1.514830	-2.380144	-0.543695
H	-3.250786	-2.519838	-0.882216
H	-2.084528	-2.332862	-2.202881
H	-1.840465	1.151718	1.475233
O	-2.447860	0.380856	1.593005
H	-1.831122	-0.408414	1.643124

4'$_{Rh}$

E= -3033.9120934au

Rh	-2.113653	-0.548756	1.485274
O	-0.683520	-1.714984	2.425568
C	0.480191	-1.798661	1.901701
C	1.520544	-2.613879	2.668833
Rh	-0.402801	-0.010872	-0.240147
O	-1.455291	1.098803	2.536838
O	-3.423300	0.665688	0.407494
O	-2.663253	-2.175083	0.296487
O	0.894373	-1.231454	0.825379
O	-1.844527	1.149547	-1.192041
O	-1.120142	-1.640440	-1.322887
O	0.157103	1.574125	0.968847
C	-0.479391	1.781041	2.065852
C	-3.020112	1.222655	-0.663705
C	-2.076392	-2.347697	-0.820322
C	-0.051342	3.022265	2.847901
C	-4.000794	2.086563	-1.454002
C	-2.507075	-3.526956	-1.690866
N	1.100893	0.477060	-1.866947
C	2.258752	-0.376949	-1.779248
C	3.353923	0.367717	-1.432153
C	2.944722	1.776799	-1.394209

C	1.573978	1.819673	−1.718171
F	2.170396	−1.797099	3.580814
F	2.471479	−3.139693	1.811861
F	0.940035	−3.655463	3.355371
F	−0.493568	2.981268	4.149797
F	−0.588098	4.150811	2.242437
F	1.321776	3.152643	2.857427
F	−4.009920	1.670156	−2.782218
F	−5.278747	2.008936	−0.966208
F	−3.594576	3.409943	−1.431046
F	−3.692439	−4.076178	−1.275772
F	−2.656639	−3.103135	−3.006902
F	−1.532108	−4.510348	−1.671785
C	0.861917	3.010579	−1.822881
C	3.624306	2.970852	−1.125390
H	4.672127	2.962947	−0.848084
C	1.564093	4.200652	−1.578332
C	2.922340	4.179134	−1.224368
H	3.436362	5.113235	−1.023703
H	−0.195473	3.023118	−2.060865
H	1.043906	5.149577	−1.653001
C	4.712584	−0.142782	−1.162693
C	5.839845	0.466411	−1.751895
C	4.909693	−1.241873	−0.301479
C	7.125216	−0.016888	−1.494892
H	5.701874	1.303917	−2.427868
C	6.197723	−1.721274	−0.046437
H	4.054786	−1.697078	0.186879
C	7.308609	−1.112315	−0.641882
H	7.982210	0.457481	−1.962537
H	6.333444	−2.563806	0.624146
H	8.307852	−1.484927	−0.440661
C	2.129035	−1.829999	−2.106316
H	1.581052	−1.974309	−3.045847
H	3.119276	−2.276903	−2.218393
H	1.595850	−2.381812	−1.325394
H	−1.590231	0.555884	−3.437982
O	−0.917557	−0.051741	−3.775567
H	−1.195541	−0.917018	−3.442839
H	0.463076	0.300879	−2.671137

$Fe(OAc)_2(THF)$

E= -812.8470846au

H	−2.611493	3.610892	1.073627
C	−2.172051	2.915268	0.353012
C	−0.994607	3.535168	−0.434571
C	−1.521313	1.710458	1.035342
H	−2.962976	2.589570	−0.332220
C	−0.220317	2.306428	−0.927648
H	−1.326459	4.169576	−1.261252
H	−0.371099	4.144170	0.230136
O	−0.494409	1.257189	0.077501
H	−2.181400	0.862169	1.217982
H	−1.014261	1.988957	1.966072
H	0.861292	2.433775	−0.979577
H	−0.588039	1.940308	−1.891644
O	2.178214	0.109734	−0.995247
C	2.770117	−0.262715	0.062241
O	2.080347	−0.809447	1.014385
C	4.258028	−0.107745	0.235266
Fe	0.321537	−0.662087	0.017762
H	4.669168	0.543874	−0.536977
H	4.483169	0.289384	1.229077
H	4.735203	−1.092224	0.162846
O	−1.503792	−1.541243	1.007400
C	−1.668621	−2.146885	−0.094873
O	−0.822929	−1.951179	−1.056499
C	−2.823431	−3.086797	−0.319499
H	−3.407456	−3.204029	0.593822
H	−3.465002	−2.701437	−1.119841
H	−2.446870	−4.060249	−0.649815

$\mathbf{1}_{Fe(OAc)2}$

E= -1446.8688628au

C	2.494417	2.036666	−0.638308
C	2.835966	1.163357	0.409963
C	3.067852	3.310198	−0.707083
H	2.798102	3.978543	−1.519018

C	3.756754	1.585489	1.382135
H	4.025503	0.915200	2.193728
C	3.989145	3.724096	0.264696
C	4.332083	2.860351	1.310128
H	4.433655	4.712770	0.207478
H	5.042600	3.176329	2.067608
C	2.219357	-0.210626	0.465275
H	1.763220	1.722458	-1.376571
N	0.705040	-0.254495	0.699552
C	1.439716	-0.614650	1.658646
C	1.335305	-1.149418	3.031336
H	1.742844	-0.429026	3.750860
H	0.287730	-1.351245	3.272398
H	1.921265	-2.070818	3.125578
C	2.781831	-1.272059	-0.448203
C	4.135878	-1.236471	-0.830790
C	1.968158	-2.318097	-0.922028
C	4.668419	-2.227458	-1.659606
H	4.770687	-0.428081	-0.484809
C	2.504360	-3.301960	-1.759982
H	0.914364	-2.355216	-0.657452
C	3.854092	-3.264734	-2.127793
H	5.715516	-2.185077	-1.943216
H	1.860629	-4.094996	-2.129142
H	4.265778	-4.031640	-2.776603
H	-6.020200	1.010671	-2.296708
C	-5.273913	1.124292	-1.504964
C	-5.796766	0.685678	-0.117994
C	-4.059014	0.211839	-1.715625
H	-4.963496	2.175358	-1.478473
C	-4.503490	0.403567	0.654701
H	-6.408232	1.453007	0.365820
H	-6.401343	-0.224609	-0.208383
O	-3.549702	-0.066753	-0.364160
H	-3.246676	0.672238	-2.281179
H	-4.333902	-0.745548	-2.172104
H	-4.584123	-0.382883	1.407076
H	-4.083266	1.305180	1.111660
Fe	-1.442380	-0.137868	0.115131
O	-1.560659	1.901497	0.752332
C	-1.225040	2.315876	-0.414863
O	-1.018867	1.477260	-1.355534
C	-1.035302	3.795074	-0.653356
H	-1.161037	4.033793	-1.711541
H	-1.734190	4.373334	-0.044201
H	-0.017815	4.075905	-0.354165
O	-1.427811	-2.209002	-0.266732
C	-1.783866	-2.506873	0.936648
O	-1.936538	-1.591002	1.802822
C	-2.015006	-3.958348	1.288940
H	-2.256041	-4.065056	2.347512
H	-2.837607	-4.356749	0.684510
H	-1.124362	-4.548517	1.048007

$TS_{(1\text{-}2)Fe(OAc)2}$

E= -1446.8424504au

N	0.423937	-0.362391	1.303958
C	1.578313	-0.658942	1.693328
C	2.462304	-0.279371	0.548601
C	2.855017	1.112981	0.387251
C	2.885813	1.985623	1.506651
H	2.600239	1.612303	2.485593
C	3.208396	1.649604	-0.878042
H	3.139423	1.021624	-1.757482
C	3.277888	3.315422	1.370847
H	3.300103	3.961187	2.243273
C	3.643405	3.819685	0.113599
H	3.949317	4.855729	0.009336
C	3.599784	2.980702	-1.008300
H	3.855501	3.370364	-1.988311
C	2.810186	-1.340289	-0.408282
C	4.090253	-1.355777	-1.018636
C	1.924838	-2.411452	-0.683490
C	4.466506	-2.400011	-1.864257
H	4.795588	-0.562197	-0.799867
C	2.307714	-3.443036	-1.542255
H	0.922223	-2.408144	-0.269218
C	3.577423	-3.447996	-2.133749

H	5.456527	-2.396937	-2.309675
H	1.604022	-4.240820	-1.757220
H	3.869332	-4.255145	-2.797931
C	2.003742	-1.344380	2.963104
H	1.136389	-1.542228	3.598319
H	2.500603	-2.292376	2.722783
H	2.725252	-0.729341	3.514440
O	-1.492808	1.954073	0.880911
C	-0.974599	2.274554	-0.253273
O	-0.715702	1.373769	-1.113447
C	-0.642541	3.721755	-0.531021
H	-0.614561	3.908488	-1.606581
H	-1.367211	4.380475	-0.046130
H	0.348098	3.947641	-0.117608
Fe	-1.429629	-0.109238	0.416192
O	-1.465296	-2.168895	-0.068798
C	-2.172310	-2.450653	0.973994
O	-2.507037	-1.534275	1.783826
C	-2.588743	-3.884494	1.207291
H	-3.176272	-3.970667	2.122329
H	-3.176717	-4.242847	0.355168
H	-1.700890	-4.522559	1.277860
O	-3.392899	0.081725	-0.490561
C	-4.506419	0.638884	0.293160
C	-3.623489	0.276211	-1.929521
C	-5.616344	0.899547	-0.731551
H	-4.756316	-0.094773	1.061189
H	-4.152117	1.559938	0.767983
C	-4.821533	1.229926	-2.015688
H	-2.701113	0.674517	-2.355074
H	-3.842770	-0.704040	-2.367538
H	-6.224585	-0.000587	-0.880637
H	-6.281464	1.711853	-0.423884
H	-5.405896	1.080578	-2.928457
H	-4.483584	2.272758	-1.995355

2 $_{Fe(OAc)2}$

E= -1446.8456127au

N	-0.298496	-0.467285	0.359633
C	-1.469110	-0.956596	0.123968
C	-2.651567	-0.112760	0.022051
C	-2.519111	1.327259	-0.216391
C	-1.440201	1.869389	-0.962163
H	-0.693057	1.215846	-1.398758
C	-3.483905	2.229766	0.304896
H	-4.307046	1.842713	0.894229
C	-1.339388	3.245471	-1.168407
H	-0.507933	3.634005	-1.748084
C	-2.296444	4.119361	-0.636671
H	-2.207945	5.189520	-0.795492
C	-3.369396	3.603473	0.102626
H	-4.110454	4.272994	0.527832
C	-3.996799	-0.700275	0.172156
C	-5.051058	-0.315955	-0.691128
C	-4.280061	-1.649694	1.181787
C	-6.325199	-0.870201	-0.558789
H	-4.854050	0.407713	-1.474182
C	-5.558421	-2.193388	1.318440
H	-3.497674	-1.936925	1.875347
C	-6.585747	-1.810338	0.446655
H	-7.114520	-0.571085	-1.241173
H	-5.755264	-2.910784	2.108801
H	-7.578013	-2.237187	0.551298
C	-1.550895	-2.476131	-0.070732
H	-0.670761	-2.793880	-0.636509
H	-1.529555	-2.996093	0.893140
H	-2.458106	-2.769146	-0.602796
O	1.664275	-1.844141	-1.462354
C	1.583899	-0.895798	-2.304298
O	1.489125	0.322625	-1.895712
C	1.582826	-1.175515	-3.788386
Fe	1.579796	-0.278916	0.147257
H	2.344677	-0.565135	-4.283795
H	1.769263	-2.232918	-3.980653
H	0.613887	-0.893253	-4.216266
O	2.173957	-0.864471	2.142220
O	3.729401	-0.261166	-0.236704
C	2.232768	0.371471	2.480196

C	4.642430	−1.344644	0.150223
C	4.468358	0.978741	−0.502182
O	2.014941	1.278106	1.607740
C	2.519899	0.746519	3.913669
H	4.652460	−2.077099	−0.663624
C	6.004143	−0.663953	0.347766
H	4.237313	−1.803456	1.053804
C	5.932929	0.541190	−0.617839
H	4.051384	1.410851	−1.413979
H	4.296344	1.662614	0.335007
H	1.583778	0.726394	4.485369
H	3.203628	0.025280	4.367985
H	2.933094	1.755513	3.970692
H	6.839161	−1.335656	0.128135
H	6.111869	−0.315327	1.381653
H	6.627609	1.342192	−0.348253
H	6.161395	0.223140	−1.642037

$TS_{(2\text{-}3)Fe(OAc)2}$

E= -1446.830501au

C	−1.409676	−0.597891	0.290950
N	−0.389905	0.200347	0.210002
C	−2.732408	−0.068468	−0.019511
C	−2.689498	1.254755	−0.549788
C	−1.431350	1.727203	−1.059235
H	−0.785934	1.061694	−1.626132
C	−3.745373	2.201950	−0.365516
H	−4.705688	1.858207	0.000977
C	−1.199843	3.118764	−1.185934
H	−0.236031	3.463336	−1.545198
C	−2.221246	4.017410	−0.923184
H	−2.054064	5.083012	−1.044757
C	−3.507130	3.551845	−0.539224
H	−4.299898	4.268211	−0.348885
C	−1.169388	−2.062745	0.647178
H	−0.362478	−2.451568	0.019152
H	−0.842197	−2.146230	1.689540
H	−2.066086	−2.668929	0.507800
C	−3.987980	−0.813743	0.169579
C	−4.992003	−0.786226	−0.826024
C	−4.243957	−1.542188	1.354219
C	−6.199605	−1.463485	−0.646458
H	−4.805207	−0.243153	−1.746476
C	−5.454255	−2.215390	1.532630
H	−3.500546	−1.552787	2.143589
C	−6.435034	−2.181146	0.533184
H	−6.953221	−1.438061	−1.427096
H	−5.635282	−2.761002	2.453152
H	−7.373248	−2.708548	0.672444
H	6.461359	−0.671145	1.023085
C	5.964262	−1.184939	0.191753
C	4.483801	−1.420007	0.510817
C	5.898575	−0.263541	−1.047868
H	6.501561	−2.118182	−0.001588
H	4.263944	−1.577563	1.568116
O	3.814549	−0.176176	0.112844
H	4.054750	−2.239321	−0.076224
C	4.689211	0.632865	−0.744324
H	6.815541	0.313802	−1.198510
H	5.719570	−0.857355	−1.952059
Fe	1.620496	0.000507	0.186713
H	4.113413	0.919523	−1.626656
H	4.967656	1.530505	−0.181285
O	1.972269	1.606382	1.500724
O	1.625328	−1.728966	−1.075184
C	2.003384	0.812438	2.510489
C	1.640575	−1.009936	−2.142377
O	1.836236	−0.440174	2.347489
C	2.220158	1.386006	3.891648
O	1.668270	0.259307	−2.064477
C	1.596579	−1.698158	−3.488915
H	2.396289	0.589513	4.616303
H	3.065649	2.080631	3.880854
H	1.333806	1.956649	4.193139
H	1.813758	−0.990385	−4.290429
H	2.310073	−2.527263	−3.512936
H	0.598951	−2.124420	−3.650162

$\mathbf{3}_{\mathbf{Fe(OAc)2}}$

E= -1446.8904561au

N	0.509878	0.325633	0.054961
C	1.495720	−0.365253	0.580443
C	2.812800	0.044606	0.065861
C	2.574492	1.057464	−0.836695
C	1.085628	1.208545	−0.952589
H	0.772441	0.710506	−1.899781
C	0.609468	2.621969	−1.132336
C	3.420640	2.008286	−1.508724
H	4.488749	1.835723	−1.581367
C	1.468887	3.517169	−1.678803
C	2.867075	3.187378	−1.926304
H	3.495985	3.941630	−2.389715
H	−0.428048	2.848066	−0.908487
H	1.132513	4.521956	−1.915147
C	4.123800	−0.517824	0.453123
C	5.050177	−0.904804	−0.537326
C	4.491989	−0.659486	1.806983
C	6.302549	−1.415726	−0.185712
H	4.772043	−0.820595	−1.583140
C	5.743931	−1.173470	2.156461
H	3.803302	−0.343917	2.583917
C	6.653502	−1.553761	1.162446
H	6.999988	−1.713273	−0.962573
H	6.011490	−1.270539	3.203981
H	7.624753	−1.953659	1.435586
C	1.228760	−1.484146	1.544516
H	2.147271	−1.983296	1.856012
H	0.708793	−1.105048	2.431784
H	0.564976	−2.217233	1.071377
Fe	−1.623011	−0.151072	0.017785
O	−1.262371	−2.258620	−0.509265
C	−1.217261	−1.924843	−1.742842
O	−1.357453	−0.699650	−2.085633
C	−1.032998	−2.985103	−2.804856
H	−0.480163	−3.837339	−2.403802
H	−2.016864	−3.342014	−3.134713
H	−0.518344	−2.569843	−3.674339
O	−2.194587	1.971263	0.428123
C	−2.161847	1.689482	1.674622
O	−1.928155	0.490694	2.059999
C	−2.360662	2.779160	2.703615
H	−2.968013	3.588859	2.293486
H	−2.822871	2.372982	3.606297
H	−1.383992	3.193847	2.983623
H	−3.915971	−2.538983	0.680997
C	−4.344770	−1.549921	0.852923
C	−5.850299	−1.451349	0.582892
O	−3.728081	−0.637676	−0.119034
H	−4.077906	−1.203217	1.857100
C	−6.012696	0.011946	0.111503
H	−6.447094	−1.679355	1.470985
H	−6.146231	−2.144264	−0.213674
C	−4.739308	0.250057	−0.711517
H	−6.921682	0.171046	−0.476065
H	−6.043994	0.687235	0.974708
H	−4.351736	1.268658	−0.653020
H	−4.862557	−0.039838	−1.760800

$\mathbf{TS}_{\mathbf{(2\text{-}4)Fe(OAc)2}}$

E= -1446.7897592au

C	1.220502	−0.589526	0.062466
N	0.163024	0.224433	0.101933
C	2.545056	−0.069481	0.007970
C	2.749370	1.375513	−0.005038
C	1.642109	2.235603	0.054772
H	0.508844	1.315608	0.077021
C	4.019682	2.008155	−0.111267
H	4.914824	1.401294	−0.184847
C	1.700899	3.614772	0.039408
H	0.804014	4.224032	0.091488
C	2.974521	4.209453	−0.051355
H	3.067070	5.291163	−0.067022
C	4.118076	3.399590	−0.128932
H	5.097187	3.861369	−0.209343
C	3.725965	−0.977045	−0.043000

C	4.657811	-0.999993	1.015018
C	3.950895	-1.817315	-1.151976
C	5.773168	-1.842088	0.968191
H	4.495168	-0.362337	1.878122
C	5.068250	-2.656673	-1.198998
H	3.247686	-1.802906	-1.978593
C	5.982726	-2.672489	-0.139204
H	6.474873	-1.852201	1.796453
H	5.225558	-3.294629	-2.063122
H	6.849103	-3.325254	-0.175783
C	0.920910	-2.076020	0.093422
H	1.825797	-2.670644	0.214153
H	0.235907	-2.287772	0.919691
H	0.418176	-2.373525	-0.834236
O	-1.613673	-1.111281	1.821342
C	-1.854216	-0.108997	2.605188
O	-2.012423	1.046067	2.121519
C	-1.911954	-0.361560	4.093609
Fe	-1.662825	-0.032364	0.117776
H	-2.323173	0.506556	4.610880
H	-2.515562	-1.249065	4.305412
H	-0.901024	-0.555316	4.471502
O	-1.644593	-1.079351	-1.949268
O	-3.658659	-0.306911	0.136111
C	-1.788736	0.099253	-2.388226
C	-4.300478	-1.592753	-0.185553
C	-4.611204	0.809149	0.025857
O	-1.881080	1.088982	-1.565219
C	-1.821549	0.387045	-3.871575
H	-4.355939	-2.170729	0.742053
C	-5.681265	-1.209733	-0.731832
H	-3.661181	-2.104079	-0.906802
C	-5.983168	0.129673	-0.019734
H	-4.447288	1.448894	0.894436
H	-4.378591	1.362558	-0.888672
H	-0.824921	0.706479	-4.200354
H	-2.098273	-0.509991	-4.428678
H	-2.517402	1.201337	-4.089119
H	-6.433386	-1.977032	-0.527167
H	-5.634497	-1.060641	-1.816817
H	-6.724468	0.732652	-0.552025
H	-6.356991	-0.052621	0.994503

$TS_{(3\text{-}4)Fe(OAc)2}$

E= -1446.8601349au

N	0.520268	0.394518	0.279298
C	1.602999	-0.325901	0.735871
C	2.803469	0.083444	0.128890
C	2.476641	1.101463	-0.810702
C	1.052728	1.298985	-0.726600
H	0.393730	0.260356	-1.087087
C	0.417681	2.427571	-1.339902
C	3.236292	1.946029	-1.660553
H	4.308805	1.812323	-1.748162
C	1.196694	3.214775	-2.162890
C	2.592704	2.970282	-2.331872
H	3.163754	3.628328	-2.979329
H	-0.633987	2.622824	-1.164415
H	0.745339	4.055600	-2.679697
C	4.155846	-0.462138	0.382306
C	4.991837	-0.834787	-0.690450
C	4.648057	-0.606889	1.695177
C	6.274524	-1.338672	-0.457148
H	4.622608	-0.743792	-1.706998
C	5.929975	-1.114187	1.926972
H	4.028537	-0.299623	2.531240
C	6.748404	-1.481600	0.852466
H	6.901088	-1.624950	-1.296335
H	6.292255	-1.214476	2.945467
H	7.744332	-1.873339	1.033403
C	1.382751	-1.444330	1.712159
H	0.580581	-2.103132	1.361133
H	2.291285	-2.037075	1.840650
H	1.084183	-1.060456	2.695788
Fe	-1.665471	-0.081752	0.409658
O	-2.288602	2.075728	0.489416
C	-2.233390	1.951808	1.755917
O	-1.930959	0.813702	2.275963

O	-1.314269	-2.181210	-0.111348
C	-1.123873	-1.891365	-1.338927
O	-1.179120	-0.666253	-1.725489
C	-2.488281	3.131617	2.661833
H	-1.529751	3.526203	3.020758
H	-3.012330	3.923436	2.123905
H	-3.063437	2.819286	3.537527
C	-0.793906	-2.977555	-2.334781
H	-1.146430	-3.946861	-1.977534
H	-1.231141	-2.745546	-3.308841
H	0.294381	-3.034049	-2.463955
H	-4.155592	0.024119	-1.822394
C	-4.590067	0.165784	-0.826646
C	-5.972457	-0.483547	-0.696343
O	-3.743425	-0.554126	0.139052
H	-4.552572	1.223340	-0.562627
C	-5.630520	-1.938087	-0.300411
H	-6.547800	-0.420605	-1.624554
H	-6.553183	0.000983	0.097387
C	-4.424079	-1.760628	0.629471
H	-6.461583	-2.451541	0.191755
H	-5.349836	-2.517886	-1.187595
H	-3.700021	-2.576056	0.593440
H	-4.726021	-1.578652	1.667088

4$_{\mathbf{Fe(OAc)2}}$

E= -1446.9355169au

H	5.340778	-2.722390	-2.271362
C	4.589154	-2.523429	-1.502016
C	5.189349	-2.452321	-0.079444
C	3.940856	-1.144228	-1.666040
H	3.829545	-3.311879	-1.555587
C	4.135952	-1.651692	0.694596
H	5.358334	-3.440594	0.357896
H	6.147521	-1.919579	-0.095509
O	3.528237	-0.754071	-0.306795
H	3.045191	-1.139442	-2.289573
H	4.651905	-0.392988	-2.027606
H	4.537184	-1.024422	1.492254
H	3.339098	-2.285848	1.095473
O	2.487708	0.982158	2.083129
C	2.794947	1.994220	1.384738
O	2.402470	2.064901	0.153831
C	3.626845	3.118046	1.951705
Fe	1.621244	0.139104	0.140404
H	3.713828	3.023681	3.034990
H	4.629223	3.087638	1.508049
H	3.187139	4.084831	1.689222
O	0.659287	-0.950654	-1.507791
C	0.373474	-1.867754	-0.671099
O	0.774459	-1.757878	0.548691
C	-0.455356	-3.058625	-1.079105
H	-0.437693	-3.186132	-2.162828
H	-0.096668	-3.962912	-0.580648
H	-1.493275	-2.895938	-0.763109
C	-1.518876	0.446953	1.266962
N	-0.484644	1.296715	0.773522
C	-2.561203	0.438004	0.371712
C	-2.237082	1.383177	-0.692976
C	-0.974827	1.940553	-0.386193
H	0.046232	1.834650	1.450924
C	-2.927149	1.831254	-1.832258
H	-3.900733	1.424507	-2.083116
C	-0.381417	2.933252	-1.169917
H	0.597579	3.329216	-0.924976
C	-1.089373	3.368579	-2.294979
H	-0.659276	4.138703	-2.927572
C	-2.345810	2.823178	-2.623509
H	-2.869692	3.182755	-3.503557
C	-3.791796	-0.382279	0.438270
C	-4.211468	-1.121897	-0.687811
C	-4.580850	-0.438167	1.604639
C	-5.371687	-1.900383	-0.642304
H	-3.615482	-1.089409	-1.594372
C	-5.738591	-1.221139	1.650029
H	-4.294338	0.153794	2.467542
C	-6.138360	-1.955921	0.527874
H	-5.675205	-2.465371	-1.518441

H	−6.333710	−1.248662	2.557745
H	−7.039484	−2.560005	0.562821
C	−1.301641	−0.304456	2.541521
H	−2.143227	−0.971157	2.740321
H	−0.394192	−0.914162	2.479646
H	−1.198278	0.372207	3.401331

T-Fe(OAc)$_2$(THF)

E= -812.8184275au

H	−2.952543	3.066787	1.262246
C	−2.491049	2.334553	0.593390
C	−1.806915	2.983880	−0.630926
C	−1.335721	1.578689	1.265792
H	−3.270201	1.635846	0.266363
C	−0.811795	1.902777	−1.066003
H	−2.513950	3.241598	−1.424864
H	−1.279514	3.897877	−0.333597
O	−0.406706	1.236109	0.179447
H	−1.634444	0.649097	1.755587
H	−0.793412	2.206554	1.981838
H	0.095207	2.284456	−1.538782
H	−1.273457	1.155301	−1.721076
O	2.067321	0.006052	−1.062068
C	2.740020	0.105431	0.028473
O	2.169787	−0.329441	1.092570
C	4.129889	0.667747	0.050102
Fe	0.562817	−0.775425	−0.005412
H	4.252533	1.408517	−0.743025
H	4.344419	1.111093	1.024475
H	4.853626	−0.138261	−0.124460
O	−0.831918	−1.799776	1.007393
C	−1.436034	−2.028436	−0.102746
O	−0.900929	−1.536585	−1.160535
C	−2.693761	−2.844674	−0.162444
H	−3.090003	−3.008885	0.840382
H	−3.439701	−2.344333	−0.787437
H	−2.480040	−3.815293	−0.625236

T-1$_{Fe(OAc)2}$

E= -1446.8402948au

C	2.574452	1.906173	−0.684471
C	2.689717	1.097934	0.461051
C	3.182720	3.164690	−0.720315
H	3.084183	3.783669	−1.606637
C	3.426238	1.568109	1.560164
H	3.527403	0.946239	2.444963
C	3.917606	3.627088	0.380064
C	4.038161	2.826855	1.520987
H	4.391411	4.603199	0.347279
H	4.606149	3.178656	2.376558
C	2.045605	−0.263597	0.486696
H	1.985492	1.557637	−1.526100
N	0.532942	−0.311786	0.715898
C	1.259828	−0.682464	1.677197
C	1.141496	−1.236588	3.041359
H	1.543671	−0.531544	3.778699
H	0.090480	−1.439163	3.267070
H	1.722088	−2.162503	3.125418
C	2.612484	−1.321207	−0.429132
C	3.983894	−1.317181	−0.746004
C	1.792471	−2.335044	−0.957160
C	4.527337	−2.308364	−1.567366
H	4.623913	−0.534500	−0.353385
C	2.340960	−3.318953	−1.787283
H	0.728481	−2.348462	−0.733374
C	3.706771	−3.313063	−2.092302
H	5.587573	−2.291972	−1.800106
H	1.694583	−4.088316	−2.199479
H	4.126899	−4.080021	−2.735672
H	−5.732484	1.052412	−2.326294
C	−4.986508	1.212324	−1.542392
C	−5.524764	0.898210	−0.127554
C	−3.789144	0.261995	−1.681972
H	−4.654880	2.255573	−1.597315
C	−4.241985	0.653881	0.670413
H	−6.119765	1.716703	0.288048
H	−6.148482	−0.003285	−0.145019

O	-3.331123	0.018912	-0.298311
H	-2.949699	0.679792	-2.240641
H	-4.068780	-0.710332	-2.099215
H	-4.339408	-0.043698	1.502996
H	-3.775307	1.582095	1.013273
Fe	-1.361657	-0.102492	0.150239
O	-1.369190	1.852625	0.543820
C	-0.961581	2.295854	-0.602604
O	-0.714653	1.496648	-1.546623
C	-0.766643	3.788831	-0.756039
H	-0.797465	4.069679	-1.810908
H	-1.526719	4.337144	-0.193362
H	0.214398	4.065971	-0.351648
O	-1.455590	-2.057290	-0.213437
C	-1.931366	-2.460736	0.923332
O	-2.115845	-1.648756	1.868936
C	-2.249050	-3.934417	1.066566
H	-2.586729	-4.154872	2.080325
H	-3.030759	-4.215799	0.352085
H	-1.364742	-4.536116	0.830466

T-TS$_{(1\text{-}2)Fe(OAc)2}$

E= -1446.8177136au

N	0.501817	-0.113263	0.114286
C	1.247877	-0.193296	1.126337
C	2.531510	0.039769	0.407103
C	2.996042	1.404821	0.187015
C	2.454170	2.478624	0.941289
H	1.675000	2.281108	1.670993
C	3.981530	1.715044	-0.784651
H	4.384227	0.923235	-1.404263
C	2.895159	3.786317	0.749692
H	2.470361	4.588938	1.345313
C	3.884819	4.067949	-0.203637
H	4.227463	5.087089	-0.351215
C	4.419512	3.025536	-0.971291
H	5.170358	3.236678	-1.726115
C	3.261594	-1.153017	-0.079547
C	4.663901	-1.241616	0.089125
C	2.585733	-2.256920	-0.645891
C	5.358975	-2.391741	-0.292239
H	5.200614	-0.415546	0.542472
C	3.289734	-3.398530	-1.034162
H	1.515398	-2.195689	-0.807077
C	4.677056	-3.475294	-0.857975
H	6.433247	-2.441277	-0.143307
H	2.752579	-4.228081	-1.483323
H	5.219196	-4.365875	-1.159391
C	1.009839	-0.493574	2.574924
H	-0.022506	-0.809751	2.734216
H	1.689108	-1.290302	2.902277
H	1.221727	0.387667	3.193511
O	-1.697423	1.584222	0.869756
C	-1.644269	2.151239	-0.284712
O	-1.608667	1.394148	-1.311211
C	-1.568613	3.647716	-0.405846
H	-1.973852	3.974271	-1.365971
H	-2.101211	4.127935	0.418414
H	-0.516326	3.955606	-0.357836
Fe	-1.550366	-0.217089	-0.019537
O	-1.512989	-2.072910	-0.861025
C	-1.681663	-2.567659	0.303792
O	-1.726474	-1.745880	1.292368
C	-1.848837	-4.046030	0.518892
H	-1.549219	-4.597257	-0.373875
H	-1.259506	-4.372333	1.380614
H	-2.900656	-4.267992	0.735831
O	-3.803263	-0.361292	-0.228117
C	-4.653636	0.065443	0.890562
C	-4.464043	-0.078201	-1.508772
C	-6.022759	0.367263	0.266475
H	-4.665493	-0.745527	1.622446
H	-4.197967	0.951601	1.344521
C	-5.648497	0.831575	-1.159057
H	-3.724273	0.386325	-2.162399
H	-4.790676	-1.031852	-1.939822
H	-6.636764	-0.540266	0.221646
H	-6.577580	1.124207	0.828871

H	−6.473797	0.733789	−1.870567
H	−5.332924	1.881650	−1.146708

T-2$_{Fe(OAc)2}$

E= -1446.8307921au

N	0.134991	0.080454	−0.054881
C	1.173984	−0.524756	0.431564
C	2.508761	−0.042693	0.110105
C	2.724780	1.290308	−0.470256
C	1.836378	2.374421	−0.245807
H	0.959304	2.230965	0.373116
C	3.856905	1.536286	−1.291791
H	4.544636	0.725241	−1.500306
C	2.075502	3.627398	−0.809662
H	1.379401	4.438018	−0.615493
C	3.198003	3.845289	−1.619215
H	3.376378	4.821754	−2.058795
C	4.086217	2.789307	−1.858267
H	4.954219	2.939837	−2.492943
C	3.682605	−0.913828	0.347520
C	4.840741	−0.409611	0.984290
C	3.690460	−2.267238	−0.060385
C	5.949393	−1.226849	1.214089
H	4.856093	0.625922	1.306464
C	4.803400	−3.081044	0.163548
H	2.822622	−2.670776	−0.571042
C	5.937122	−2.566438	0.804552
H	6.822063	−0.819705	1.715491
H	4.788234	−4.114929	−0.167488
H	6.800591	−3.200068	0.980697
C	0.963553	−1.722303	1.361415
H	0.184404	−1.466146	2.083567
H	0.609088	−2.589940	0.795235
H	1.876521	−1.992754	1.892986
O	−1.651347	0.044683	2.038083
C	−1.807765	1.319488	1.998061
O	−1.852035	1.861356	0.842861
C	−1.898914	2.129028	3.260187
Fe	−1.652658	−0.008141	0.038943
H	−2.409470	3.074967	3.069694
H	−2.419494	1.564282	4.037392
H	−0.888757	2.349962	3.626463
O	−1.659371	−1.881225	−0.681388
O	−3.733254	−0.090739	0.202124
C	−1.814191	−1.413758	−1.870207
C	−4.474160	−1.269509	0.676322
C	−4.595219	0.782204	−0.609172
O	−1.910381	−0.147824	−1.988259
C	−1.840891	−2.325638	−3.064038
H	−4.588092	−1.172150	1.760871
C	−5.817415	−1.214887	−0.063354
H	−3.871412	−2.150433	0.450227
C	−6.017690	0.298096	−0.310454
H	−4.387637	1.808161	−0.301102
H	−4.316252	0.654561	−1.659371
H	−0.816546	−2.475293	−3.426953
H	−2.249357	−3.301852	−2.792921
H	−2.422980	−1.878005	−3.872408
H	−6.628452	−1.661282	0.519250
H	−5.752558	−1.749573	−1.018405
H	−6.706170	0.504623	−1.134990
H	−6.410464	0.783439	0.590773

T-TS$_{(2-3)Fe(OAc)2}$

E= -1446.8143458au

C	1.293945	−0.592252	0.271714
N	0.261318	0.019924	−0.279071
C	2.590382	0.001721	0.051977
C	2.504007	1.276681	−0.565050
C	1.205767	1.904215	−0.507048
H	0.679383	1.953718	0.440538
C	3.486271	1.803464	−1.460787
H	4.467917	1.344875	−1.497933
C	0.869275	2.902044	−1.467537
H	−0.116606	3.352112	−1.429363
C	1.822391	3.335960	−2.366772
H	1.580158	4.121168	−3.076653
C	3.145785	2.805091	−2.345648

H	3.878467	3.172524	-3.056792
C	1.073367	-1.834358	1.114869
H	0.464689	-1.556507	1.982574
H	0.504749	-2.580021	0.551692
H	2.010919	-2.269680	1.463549
C	3.876653	-0.649859	0.367167
C	4.905037	0.084502	0.998192
C	4.128830	-1.996854	0.025416
C	6.135502	-0.509583	1.287801
H	4.721113	1.117679	1.273821
C	5.362117	-2.586924	0.310990
H	3.362262	-2.568641	-0.486109
C	6.367950	-1.847551	0.946249
H	6.909508	0.067909	1.783228
H	5.540487	-3.620889	0.033560
H	7.323819	-2.309483	1.171627
H	-5.496293	-1.790671	-0.716404
C	-5.596107	-1.202507	0.203169
C	-4.272240	-1.192872	0.976575
C	-5.813903	0.289791	-0.136585
H	-6.414350	-1.628274	0.791303
H	-3.654404	-2.077829	0.818400
O	-3.531365	-0.034526	0.440229
H	-4.414357	-1.020043	2.048342
C	-4.393351	0.779597	-0.434393
H	-6.486086	0.435123	-0.987314
H	-6.235247	0.820789	0.725144
Fe	-1.509277	-0.085291	0.091188
H	-4.204374	1.822257	-0.174613
H	-4.087877	0.589422	-1.467156
O	-1.960259	-0.573258	-1.803753
O	-1.279585	0.235946	2.015446
C	-1.909323	-1.860596	-1.698366
C	-1.521250	1.511690	2.080964
O	-1.695079	-2.405386	-0.580790
C	-2.084774	-2.683151	-2.957324
O	-1.697987	2.187251	1.037234
C	-1.584836	2.134411	3.459662
H	-1.141898	-2.690961	-3.517960
H	-2.350033	-3.712177	-2.707581
H	-2.846725	-2.239168	-3.603679
H	-2.463399	1.755379	3.994724
H	-0.703346	1.852629	4.044167
H	-1.651290	3.220687	3.383149

THF

E= -232.3963861au

H	1.872236	-0.571307	-0.834500
C	1.200904	-0.403985	0.013493
C	0.697764	1.064981	0.111050
O	0.034508	-1.241318	-0.196272
H	1.721785	-0.709130	0.931880
C	-0.816499	0.953638	-0.200207
H	1.215628	1.728110	-0.588110
H	0.856062	1.460905	1.120513
C	-1.125483	-0.490992	0.217683
H	-1.416284	1.694983	0.336655
H	-0.999372	1.076689	-1.273649
H	-1.993312	-0.927782	-0.282956
H	-1.272923	-0.563773	1.308224

$FeCl_2(THF)_3$

E= -850.7402387au

Fe	0.016376	-0.290534	0.121162
H	-1.913216	1.943748	-0.782704
C	-1.041038	2.401371	-1.251991
C	-0.846118	3.874665	-0.850076
O	0.140814	1.677568	-0.735817
H	-1.079416	2.249125	-2.334427
C	0.158399	3.795831	0.321281
H	-1.790346	4.346542	-0.563390
H	-0.419913	4.451487	-1.679127
C	1.061518	2.638004	-0.096524
H	0.712437	4.727736	0.467106
H	-0.351725	3.542170	1.256644
H	1.539834	2.113193	0.728897
H	1.809114	2.941797	-0.840058

O	-2.272350	-0.262185	-0.016972
C	-3.068786	-0.600018	1.187261
C	-2.962253	-0.778974	-1.207410
C	-4.249779	-1.456341	0.692283
H	-2.402539	-1.129698	1.868406
H	-3.377572	0.335377	1.660967
C	-3.780118	-1.960680	-0.690480
H	-3.602479	0.016105	-1.614941
H	-2.192081	-1.058222	-1.925728
H	-5.155676	-0.847524	0.586738
H	-4.474986	-2.273674	1.383447
H	-4.610953	-2.220306	-1.353434
H	-3.129099	-2.835119	-0.587351
Cl	-0.032983	0.232349	2.393215
O	2.250464	-0.266708	0.126067
C	2.879864	-1.183395	1.091771
C	3.015306	-0.277562	-1.134576
C	4.334319	-1.275957	0.630623
H	2.722911	-0.751389	2.079530
H	2.371984	-2.152689	1.029183
C	4.189611	-1.245619	-0.907537
H	2.346343	-0.600483	-1.934471
H	3.349806	0.749693	-1.315509
H	4.827242	-2.183948	0.990464
H	4.907679	-0.410933	0.985019
H	3.932285	-2.242901	-1.280548
H	5.100655	-0.915820	-1.415697
Cl	0.112804	-2.174567	-1.231638

CuCl(THF)

E= -443.5946872au

H	-3.889921	-1.332630	0.274246
C	-3.121019	-0.738659	-0.226989
C	-3.121392	0.738775	0.226041
C	-1.707590	-1.207729	0.132080
H	-3.286689	-0.808566	-1.307769
H	-3.888903	1.332886	-0.277143
C	-1.706901	1.208170	-0.129312
H	-3.290106	0.808594	1.306360
O	-0.869716	-0.000418	-0.001193
H	-1.630428	-1.556401	1.167110
H	-1.301704	-1.965173	-0.541322
H	-1.301564	1.962421	0.548046
H	-1.627854	1.561248	-1.162626
Cu	1.069806	-0.000172	-0.000613
Cl	3.181878	0.000153	0.000558

$\mathbf{1}_{Cu}$

E= -1077.6172836au

N	-0.093142	-0.032639	-0.222391
C	-0.440727	-0.087689	-1.436018
C	-1.603850	-0.030562	-0.516084
C	-2.312186	1.286023	-0.318380
C	-3.706175	1.370368	-0.489145
H	-4.271917	0.475394	-0.736941
C	-1.598427	2.453452	0.008263
H	-0.523728	2.406836	0.148301
C	-4.367915	2.592860	-0.338306
H	-5.443807	2.641318	-0.476065
C	-3.649234	3.747275	-0.005761
H	-4.164267	4.694576	0.117188
C	-2.263318	3.672270	0.170639
H	-1.698155	4.559798	0.436231
C	-2.335568	-1.294386	-0.155262
C	-2.851980	-1.453022	1.144155
C	-2.489392	-2.338842	-1.081198
C	-3.497089	-2.637363	1.509274
H	-2.741543	-0.649139	1.864846
C	-3.141217	-3.522603	-0.717362
H	-2.104771	-2.225267	-2.090323
C	-3.644146	-3.674785	0.579094
H	-3.881835	-2.752270	2.517404
H	-3.255791	-4.321021	-1.443553
H	-4.146610	-4.593583	0.863774
C	0.151414	-0.086576	-2.788603
H	-0.213756	0.779450	-3.354141
H	1.241816	-0.049684	-2.707435
H	-0.150535	-0.982295	-3.344110

H	5.861934	-1.740831	-0.550275
C	5.086384	-0.992996	-0.358951
C	5.402121	0.381217	-0.988002
C	3.748120	-1.352454	-1.016675
H	4.951549	-0.887448	0.722217
H	6.094229	0.973379	-0.382439
C	4.010907	1.025536	-1.073208
H	5.838495	0.258914	-1.987289
O	3.060854	-0.080687	-1.250440
H	3.889995	-1.858268	-1.982136
H	3.107235	-1.968752	-0.379800
H	3.895030	1.707872	-1.921434
H	3.758446	1.545670	-0.143474
Cu	1.335246	0.103398	1.048643
Cl	2.847922	0.324378	2.541662

$\mathbf{2_{Cu}}$

E= -1077.5816775au

C	-0.723936	-0.680518	-0.227400
N	0.347995	0.049589	-0.153894
C	-2.032461	-0.064736	-0.036368
C	-2.067749	1.372854	0.001686
C	-1.023354	2.140306	-0.591726
H	-0.399516	1.694550	-1.355575
C	-3.054188	2.061772	0.773997
H	-3.853520	1.494413	1.235846
C	-0.917185	3.516141	-0.333798
H	-0.113847	4.084082	-0.791225
C	-1.863649	4.152378	0.464979
H	-1.789830	5.219290	0.650881
C	-2.943238	3.421530	1.008583
H	-3.678220	3.925133	1.627708
C	-0.608991	-2.169445	-0.585004
H	0.137284	-2.280150	-1.377352
H	-0.253857	-2.744023	0.278620
H	-1.553691	-2.602957	-0.920947
C	-3.284484	-0.836373	0.009244
C	-4.425972	-0.398308	-0.704684
C	-3.395944	-2.010842	0.791356
C	-5.624840	-1.110030	-0.645318
H	-4.352353	0.490280	-1.321756
C	-4.600935	-2.710845	0.861287
H	-2.542186	-2.350003	1.366529
C	-5.716980	-2.266594	0.139708
H	-6.483925	-0.767761	-1.212804
H	-4.671763	-3.600543	1.478214
H	-6.650004	-2.818589	0.187771
Cl	3.678252	0.110201	-2.281818
Cu	2.067744	-0.191549	-0.819169
O	3.184120	-1.166788	0.874084
C	3.088861	-0.509028	2.171001
C	4.606537	-1.437341	0.671516
C	4.316598	0.423834	2.244082
H	2.125785	0.003399	2.200959
H	3.118607	-1.275723	2.958450
C	5.331460	-0.198616	1.232948
H	4.865775	-2.354033	1.219559
H	4.748073	-1.576035	-0.399917
H	4.718248	0.476100	3.261049
H	4.047572	1.439616	1.938935
H	5.540802	0.502101	0.420653
H	6.279470	-0.467302	1.709265

$\mathbf{TS_{(2\text{-}3)Cu}}$

E= -1077.5816529au

C	-0.746249	-0.675593	-0.243270
N	0.327595	0.052267	-0.169645
C	-2.051857	-0.050289	-0.057889
C	-2.047760	1.381384	-0.027302
C	-0.948339	2.096744	-0.593856
H	-0.377984	1.652450	-1.399826
C	-3.012159	2.115297	0.733864
H	-3.852897	1.587829	1.168770
C	-0.759654	3.459466	-0.296555
H	0.084310	3.987395	-0.727948
C	-1.681499	4.132123	0.496597
H	-1.547454	5.188130	0.709336
C	-2.821700	3.458857	0.997835

H	−3.537315	3.996587	1.610901
C	−0.632774	−2.165372	−0.589778
H	0.097401	−2.282889	−1.396165
H	−0.259276	−2.731063	0.271787
H	−1.583815	−2.602295	−0.902400
C	−3.312757	−0.805670	0.004162
C	−4.452878	−0.358200	−0.705390
C	−3.433440	−1.972925	0.794963
C	−5.660669	−1.053547	−0.632263
H	−4.371575	0.524652	−1.329917
C	−4.646376	−2.658167	0.876473
H	−2.580223	−2.318728	1.367171
C	−5.761842	−2.204203	0.160264
H	−6.519441	−0.703706	−1.195635
H	−4.723831	−3.543555	1.498815
H	−6.701349	−2.744131	0.218079
Cl	3.676197	0.089723	−2.280525
Cu	2.051984	−0.196962	−0.832212
O	3.145011	−1.194889	0.876709
C	3.044983	−0.543483	2.175944
C	4.566770	−1.473309	0.682746
C	4.279098	0.380160	2.264047
H	2.085573	−0.023888	2.201480
H	3.062893	−1.314033	2.960069
C	5.294544	−0.240070	1.252200
H	4.817955	−2.392863	1.229933
H	4.714781	−1.609892	−0.388110
H	4.675949	0.419644	3.283491
H	4.019112	1.400857	1.967534
H	5.507564	0.463969	0.443696
H	6.240806	−0.513830	1.729090

$\mathbf{3}_{\mathbf{Cu}}$

E= -1077.6400158au

N	−0.134604	0.724063	−0.601540
C	0.749766	−0.244406	−0.726033
C	2.085362	0.154435	−0.257743
C	1.975863	1.458661	0.168829
C	0.579657	1.916310	−0.145530
H	0.651802	2.528547	−1.072411
C	−0.012721	2.862035	0.859457
C	2.837864	2.331521	0.920750
H	3.891851	2.099983	1.024199
C	0.833247	3.597630	1.620657
C	2.273992	3.371248	1.606864
H	2.897394	4.011463	2.222909
H	−1.087213	3.017146	0.862011
H	0.443374	4.363525	2.283472
C	3.293661	−0.696365	−0.230825
C	4.515970	−0.207953	−0.736456
C	3.263824	−1.993608	0.320686
C	5.671990	−0.991825	−0.690921
H	4.547794	0.780507	−1.183785
C	4.421237	−2.775834	0.363990
H	2.338255	−2.378113	0.736348
C	5.628487	−2.278568	−0.141264
H	6.602781	−0.602058	−1.090586
H	4.381676	−3.770136	0.797215
H	6.525606	−2.888157	−0.108210
C	0.378421	−1.569571	−1.317843
H	1.254485	−2.195476	−1.492527
H	−0.324200	−2.089010	−0.654764
H	−0.142556	−1.419396	−2.270223
Cu	−2.017456	0.699534	−1.023391
Cl	−4.081650	0.906639	−1.549919
H	−3.809659	−1.958898	−0.878061
C	−3.608602	−2.312964	0.134545
C	−4.611674	−1.781907	1.163080
O	−2.313646	−1.764906	0.539521
H	−3.552158	−3.411172	0.146178
C	−3.770051	−1.748041	2.457634
H	−5.500546	−2.414183	1.250591
H	−4.926339	−0.773800	0.874193
C	−2.369937	−1.362374	1.942792
H	−4.151502	−1.034781	3.194585
H	−3.749077	−2.739258	2.927113
H	−1.562319	−1.866164	2.486593
H	−2.201925	−0.279646	1.990727

$TS_{(3\text{-}4)Cu}$

E= -1077.6060227au

N	−0.150073	0.649885	−0.526511
C	0.813503	−0.325121	−0.689498
C	2.060954	0.085681	−0.188181
C	1.920081	1.423192	0.275481
C	0.549740	1.800698	0.053696
C	−0.009690	2.986734	0.631386
C	2.778541	2.339820	0.936844
H	3.819278	2.088153	1.105851
C	0.865740	3.846847	1.259649
C	2.251625	3.530297	1.403436
H	2.895290	4.235004	1.919459
H	−1.067615	3.204362	0.528085
H	0.495159	4.779986	1.670391
C	3.312426	−0.705916	−0.180497
C	4.509829	−0.156976	−0.681954
C	3.338654	−2.014173	0.341988
C	5.695481	−0.897097	−0.665682
H	4.502295	0.843577	−1.102531
C	4.525115	−2.753199	0.355630
H	2.430422	−2.440243	0.755563
C	5.707196	−2.197683	−0.147924
H	6.607140	−0.461467	−1.062241
H	4.527937	−3.758280	0.765329
H	6.627991	−2.771804	−0.136236
C	0.460849	−1.581260	−1.427782
H	1.325691	−2.241115	−1.517044
H	−0.351980	−2.111864	−0.920787
H	0.107511	−1.342953	−2.439606
Cl	−4.124987	1.020199	−1.414788
H	−3.934361	−1.097809	3.148574
C	−3.651717	−1.830594	2.387113
C	−2.250255	−1.541392	1.794121
C	−4.590145	−1.786971	1.156427
H	−3.673531	−2.821707	2.854758
O	−2.383160	−1.601703	0.336860
H	−1.505092	−2.278594	2.117242
H	−1.882132	−0.540795	2.039956
C	−3.668523	−2.221024	0.015629
H	−5.461638	−2.439044	1.269030
H	−4.937248	−0.767550	0.961614
H	−3.969589	−1.833277	−0.958141
H	−3.546276	−3.313291	−0.026838
Cu	−2.094531	0.559009	−0.846180
H	0.256306	1.767326	−1.170431

4_{Cu}

E= -1077.67797au

Cl	4.351180	0.704610	0.636642
H	−0.261124	−2.047608	−0.822649
C	0.753238	−1.974392	−1.222942
C	1.257817	−3.266868	−1.880726
O	1.666365	−1.717549	−0.097934
H	0.809018	−1.120274	−1.907407
C	2.769826	−3.242440	−1.564794
H	1.047979	−3.292601	−2.954089
H	0.785833	−4.143675	−1.421838
C	2.806963	−2.654121	−0.152203
H	3.230124	−4.233478	−1.614191
H	3.298515	−2.585261	−2.264625
H	3.705008	−2.075683	0.074249
H	2.650179	−3.420378	0.616800
Cu	2.209316	0.262011	0.553026
C	−0.701853	0.341277	1.432084
N	0.397404	1.232065	1.181755
C	−1.687315	0.559184	0.502854
C	−1.264063	1.675732	−0.341644
C	−0.003731	2.102480	0.129788
H	0.815905	1.673488	1.998171
C	−1.862778	2.363133	−1.411578
H	−2.834994	2.062852	−1.786222
C	0.680072	3.189653	−0.417140
H	1.656154	3.489068	−0.049249
C	0.063726	3.863065	−1.477072
H	0.564591	4.712055	−1.930198
C	−1.191063	3.452661	−1.969029

H	−1.642767	3.995923	−2.792631
C	−2.950217	−0.198399	0.347576
C	−3.339685	−0.682147	−0.918863
C	−3.798773	−0.441469	1.446186
C	−4.531097	−1.395965	−1.076816
H	−2.698383	−0.504581	−1.776337
C	−4.988071	−1.159331	1.287167
H	−3.534245	−0.042294	2.419792
C	−5.358420	−1.639972	0.025889
H	−4.812042	−1.763412	−2.058945
H	−5.630063	−1.332897	2.145093
H	−6.283909	−2.193057	−0.097682
C	−0.562366	−0.685686	2.510612
H	−1.438390	−1.336804	2.536070
H	0.321631	−1.311390	2.336057
H	−0.455243	−0.229120	3.504280

$TS_{(1\text{-}2)Cu'}$

E= -1077.6037039au

N	−0.359686	−0.333113	1.651140
C	0.749984	0.036653	2.124291
C	1.377426	0.250304	0.811784
C	1.334055	1.592854	0.188116
C	1.330945	2.746706	1.002321
H	1.343212	2.644668	2.082050
C	1.305688	1.756609	−1.216879
H	1.232176	0.882291	−1.854515
C	1.320519	4.022314	0.434464
H	1.323324	4.897826	1.075660
C	1.305730	4.169949	−0.957560
H	1.292167	5.161106	−1.399434
C	1.293689	3.033758	−1.778347
H	1.254762	3.141846	−2.857066
C	2.223315	−0.846913	0.279483
C	3.333476	−0.555046	−0.544768
C	2.014609	−2.191344	0.664726
C	4.193984	−1.571056	−0.968459
H	3.532786	0.467688	−0.837945
C	2.870156	−3.200783	0.228836
H	1.153038	−2.445216	1.271268
C	3.966624	−2.897309	−0.589653
H	5.041020	−1.322003	−1.599554
H	2.675622	−4.228248	0.518561
H	4.629807	−3.685658	−0.930060
C	1.252954	0.062010	3.535820
H	1.562059	1.071497	3.831801
H	0.469001	−0.285874	4.214889
H	2.130894	−0.588515	3.631604
Cl	−0.887095	−1.049898	−2.314529
Cu	−0.906718	−0.460027	−0.189826
H	−4.289832	−1.936405	−0.914240
C	−4.783374	−1.018727	−0.579656
C	−4.809245	−0.947157	0.977535
C	−3.938536	0.195656	−0.992908
H	−5.786150	−0.994330	−1.016906
C	−3.728093	0.107164	1.332401
H	−5.790499	−0.639233	1.353488
H	−4.578082	−1.921639	1.418202
O	−2.989397	0.356250	0.103040
H	−4.543649	1.110057	−1.076893
H	−3.345953	0.044858	−1.895631
H	−4.181375	1.048600	1.671340
H	−2.999342	−0.226347	2.073738

$2_{Cu'}$

E= -1077.6057381au

N	−0.671943	−0.078060	1.804245
C	0.572170	−0.060518	2.056371
C	1.191408	0.040413	0.703103
C	1.578127	1.382812	0.201440
C	1.685360	2.475127	1.093789
H	1.453126	2.340238	2.143960
C	1.851642	1.609410	−1.169456
H	1.688011	0.808309	−1.880083
C	2.082008	3.734454	0.641230
H	2.162021	4.557461	1.344114
C	2.373633	3.935594	−0.713297
H	2.678652	4.915713	−1.065639

C	2.251414	2.869284	-1.614481
H	2.446114	3.024804	-2.670441
C	1.820247	-1.216584	0.201899
C	3.059689	-1.192201	-0.474440
C	1.248599	-2.476311	0.493527
C	3.691741	-2.380691	-0.850854
H	3.539188	-0.245579	-0.687293
C	1.878730	-3.657647	0.107424
H	0.288954	-2.521929	0.997235
C	3.105462	-3.617810	-0.568810
H	4.645259	-2.334652	-1.367390
H	1.408294	-4.610878	0.325960
H	3.593576	-4.538106	-0.872261
C	1.241920	-0.239487	3.391404
H	1.913891	0.595826	3.620760
H	0.483512	-0.320705	4.175883
H	1.850656	-1.152067	3.383884
Cl	-0.765475	-0.426527	-2.294153
Cu	-0.876026	-0.004914	-0.103980
H	-4.331120	-1.696188	-1.038225
C	-4.781837	-0.748557	-0.727301
C	-4.828360	-0.649494	0.829552
C	-3.878738	0.420113	-1.152119
H	-5.775426	-0.684041	-1.181032
C	-3.771254	0.425887	1.180865
H	-5.818979	-0.355767	1.191382
H	-4.581481	-1.611748	1.288296
O	-2.965798	0.590946	-0.024156
H	-4.445805	1.352440	-1.282363
H	-3.257225	0.226897	-2.025618
H	-4.239795	1.390413	1.417600
H	-3.085388	0.149098	1.981774

Calculated imaginary frequencies of all transition states species

Sep-TS$_{(2\text{-}3)Fe}$	-511.965	For the $FeCl_2$-catalyzed system
TS$_{(2\text{-}4)Fe}$	-1059.88	For the $FeCl_2$-catalyzed system
TS$_{(3\text{-}4)Fe}$	-1435.09	For the $FeCl_2$-catalyzed system
TS$_{(1\text{-}2)Rh}$	-216.581	For the $Rh_2(OCOCF_3)_4$-catalyzed system
TS$_{(2\text{-}3)Rh}$	-86.1614	For the $Rh_2(OCOCF_3)_4$-catalyzed system
TS$_{(2\text{-}4)Rh}$	-739.641	For the $Rh_2(OCOCF_3)_4$-catalyzed system
TS$_{(3\text{-}4)Rh}$	-1494.1	For the $Rh_2(OCOCF_3)_4$-catalyzed system
TS$_{(4\text{-}5)Fe'}$	-803.635	For the $FeCl_2$-catalyzed system
TS$_{(4\text{-}5)Rh'}$	-891.409	For the $Rh_2(OCOCF_3)_4$-catalyzed system
TS$_{(5\text{-}6)Rh'}$	-397.515	For the $Rh_2(OCOCF_3)_4$-catalyzed system
TS$_{(1\text{-}2)Fe(OAc)2}$	-134.818	For the $Fe(OAc)_2$-catalyzed system
TS$_{(2\text{-}3)Fe(OAc)2}$	-319.683	For the $Fe(OAc)_2$-catalyzed system
TS$_{(2\text{-}4)Fe(OAc)2}$	-1163.41	For the $Fe(OAc)_2$-catalyzed system
TS$_{(3\text{-}4)Fe(OAc)2}$	-1377.14	For the $Fe(OAc)_2$-catalyzed system
TS$_{(2\text{-}3)Cu}$	-41.75	For the CuCl-catalyzed system
TS$_{(3\text{-}4)Cu}$	-1452.12	For the CuCl-catalyzed system
TS$_{(1\text{-}2)Cu'}$	-107.036	For the CuCl-catalyzed system