Supporting Information

Theoretical Studies of Iron(III)-Catalyzed Intramolecular C-H Amination of Azides

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Complete Reference for Ref (22):

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 03, Revision D.01*, Gaussian, Inc., Wallingford, CT, 2004.

Cartesian coordinates and electronic energies:

1(D)

E=-1753.3921013au

N	−0.835851	0.414561	−1.070255
C	−1.585018	1.643618	−1.060945
C	−2.991135	1.711010	−0.903138
C	−3.849635	0.514953	−0.666871
C	−3.542099	−0.411331	0.348383
H	−2.649519	−0.269886	0.950669
N	−1.279070	−0.539351	−1.727963
N	−1.540670	−1.495261	−2.285478
C	−0.822400	2.811826	−1.196262
H	0.250868	2.718825	−1.304224
C	−3.588427	2.986256	−0.942691
H	−4.663986	3.054164	−0.815126
C	−1.441261	4.062296	−1.212903
C	−2.832767	4.150133	−1.097401
H	−0.840532	4.958938	−1.323617
H	−3.325215	5.116878	−1.112310
C	−5.023023	0.321021	−1.421344
H	−5.265590	1.020648	−2.215432
C	−4.381989	−1.501125	0.595328
H	−4.124044	−2.204189	1.381293
C	−5.544543	−1.683158	−0.162885
C	−5.863312	−0.767461	−1.171871
H	−6.194598	−2.531065	0.028851
H	−6.759931	−0.903663	−1.768423
H	−0.062964	−4.634215	0.061370
C	0.258084	−3.600319	0.122241
C	1.065698	−3.116175	−0.891590
C	−0.174535	−2.853783	1.205327
N	1.564374	−1.818520	−0.973198
C	1.509000	−3.889569	−2.027574
C	−1.027781	−3.354555	2.257594
N	0.142183	−1.520230	1.441429
C	2.329514	−1.784103	−2.132973
C	2.284165	−3.067942	−2.794994
H	1.249751	−4.923362	−2.202500
C	−1.226042	−2.327273	3.137051
H	−1.412589	−4.362767	2.305615
C	−0.489947	−1.189141	2.634171
C	3.050311	−0.693144	−2.589296
H	2.789146	−3.296377	−3.722170
H	−1.803347	−2.327759	4.050252
C	−0.427592	0.043936	3.262662
C	3.140893	0.526831	−1.940656
H	3.603462	−0.810250	−3.514849
C	0.301126	1.130191	2.808599
H	−0.977081	0.161893	4.190284
N	2.507312	0.859612	−0.748946
C	3.936501	1.640442	−2.406667
N	1.065960	1.164798	1.648315
C	0.391545	2.396370	3.500623
C	2.914880	2.157143	−0.457366
C	3.800292	2.643883	−1.490458
H	4.522311	1.635974	−3.314300
C	1.652346	2.426216	1.625099
C	1.227349	3.193563	2.772869
H	−0.118504	2.626003	4.424767
C	2.519323	2.888171	0.650068
H	4.251088	3.625541	−1.498492
H	1.538065	4.206957	2.980906
H	2.913322	3.892700	0.759558
Fe	1.439011	−0.376648	0.419090
Cl	3.228166	−1.086711	1.568319

$TS_{12(D)}$

E=-1753.3450346au

N	−0.502487	0.426266	−0.555495
C	−0.946653	1.699848	−0.917069
C	−2.356693	1.985324	−1.002572
C	−3.414882	0.966638	−0.785620
C	−3.391014	0.086386	0.313502
H	−2.570937	0.135152	1.017971
N	−0.877437	−0.593660	−1.868463

N	−1.599536	−1.340775	−2.274761
C	−0.022939	2.732006	−1.221490
H	1.026913	2.488784	−1.204349
C	−2.749994	3.290422	−1.347418
H	−3.808911	3.521418	−1.387326
C	−0.444613	4.017640	−1.542544
C	−1.815936	4.297337	−1.602247
H	0.284820	4.791425	−1.755981
H	−2.158805	5.297429	−1.848669
C	−4.428255	−0.829218	0.510433
H	−4.392343	−1.497109	1.365199
C	−4.505289	0.896375	−1.680148
H	−4.528181	1.551353	−2.545596
C	−5.502311	−0.889785	−0.384628
C	−5.536816	−0.023850	−1.483624
H	−6.360494	−0.068894	−2.188963
H	−6.303329	−1.605669	−0.229601
H	4.779227	2.866619	−1.330951
C	3.989742	2.514672	−0.682656
C	3.245098	1.290963	−0.885449
C	3.511205	3.092411	0.461361
N	2.313421	1.137415	0.129735
C	3.441400	0.416732	−1.946360
C	2.465457	2.232134	0.966257
H	3.830650	4.010922	0.932093
Fe	1.090612	−0.438588	0.384530
C	2.795300	−0.797175	−2.116506
H	4.198161	0.684274	−2.676253
C	1.699595	2.495606	2.093601
Cl	2.699723	−1.415412	1.644208
N	−0.066547	−2.066505	0.687160
N	1.822441	−1.322159	−1.276456
N	0.323693	0.454740	2.025472
C	3.112987	−1.752747	−3.158003
C	0.703643	1.667241	2.583610
H	1.913266	3.405498	2.644244
C	−0.928655	−2.259594	1.754286
C	−0.057290	−3.258925	−0.021699
C	1.570273	−2.605800	−1.739295
C	−0.616023	−0.089113	2.886281
C	2.363582	−2.868839	−2.921160
H	3.834617	−1.584212	−3.944242
C	−0.050969	1.907066	3.795446
C	−1.492857	−3.592999	1.694303
C	−1.201083	−1.341418	2.758463
C	−0.954435	−4.208643	0.601229
C	0.697252	−3.511590	−1.156781
C	−0.863491	0.825769	3.982429
H	2.344998	−3.794875	−3.477238
H	0.053123	2.783273	4.418794
H	−2.195329	−3.993597	2.410968
H	−1.902090	−1.642667	3.529955
H	−1.130965	−5.211738	0.241162
H	0.604972	−4.489630	−1.616189
H	−1.557384	0.641036	4.789722

2(D)

E=-1643.8767267au

N	0.254101	0.679116	−0.202727
C	0.346029	1.960611	−0.547134
C	1.669182	2.565554	−0.672383
C	2.914755	1.780245	−0.528809
C	3.054661	0.499302	−1.101849
H	2.225027	0.060053	−1.643783
C	−0.809396	2.792473	−0.753415
C	1.743706	3.938975	−0.942410
H	2.721128	4.395564	−1.054208
C	0.598447	4.722794	−1.113761
H	0.700362	5.780748	−1.332898
C	−0.680980	4.142086	−1.025140
H	−1.566372	4.751607	−1.171108
H	−1.783387	2.335521	−0.675923
C	4.019695	2.334425	0.154030
H	3.922066	3.306614	0.626704
C	4.261824	−0.196942	−0.998015
H	4.348149	−1.178924	−1.451827
C	5.347049	0.364146	−0.315581
H	6.282068	−0.181173	−0.233947

C	5.220732	1.632619	0.263918
H	6.053154	2.070656	0.805368
C	1.977269	-3.463820	-1.552773
C	1.294846	-3.095414	-2.678128
C	1.405229	-2.725720	-0.445702
H	2.792880	-4.166861	-1.463640
C	0.280518	-2.145863	-2.268588
H	1.437865	-3.439807	-3.692120
N	0.370000	-1.931191	-0.904435
C	1.871743	-2.773350	0.859200
C	-0.671890	-1.591954	-3.111597
Fe	-0.779177	-0.686553	0.194379
C	1.391300	-1.995383	1.900187
H	2.697392	-3.443168	1.073120
C	-1.733693	-0.803598	-2.694536
H	-0.627120	-1.856669	-4.162355
Cl	-2.120906	-2.474343	0.726775
N	0.343744	-1.095882	1.820158
N	-1.994594	0.451084	1.317543
N	-1.960750	-0.368202	-1.399004
C	1.948705	-1.973923	3.237378
C	-2.840848	-0.407456	-3.538574
C	0.231353	-0.509044	3.066746
C	-1.800951	0.804993	2.642541
C	-3.233230	0.955765	0.951204
C	-3.199021	0.255258	-1.403523
C	1.244001	-1.048553	3.951994
H	2.774753	-2.587835	3.565702
C	-3.749077	0.229239	-2.741223
H	-2.910821	-0.621689	-4.595107
C	-0.743902	0.401519	3.444641
C	-2.931244	1.582043	3.105801
C	-3.819032	1.660594	2.070679
C	-3.805707	0.852401	-0.307995
H	1.372028	-0.758222	4.984716
H	-4.706544	0.646644	-3.017036
H	-0.721650	0.767266	4.465448
H	-3.028275	1.983977	4.103930
H	-4.783788	2.146326	2.050125
H	-4.784832	1.294973	-0.454056

$TS_{23(D)}$

E=-1643.8533407au

N	0.332788	0.907067	-0.038695
C	-0.034554	2.159682	-0.304698
C	1.031950	3.138920	-0.514905
C	2.317939	2.531785	-0.583151
C	2.299301	1.112985	-0.810754
C	-1.387228	2.658418	-0.305320
C	0.738363	4.514074	-0.618013
H	1.543525	5.223517	-0.779600
C	-0.573285	4.949265	-0.552711
H	-0.803492	6.005016	-0.649215
C	-1.628624	4.011713	-0.388038
H	-2.651845	4.370326	-0.337927
H	-2.200369	1.969319	-0.169816
C	3.533849	3.172911	-0.233681
H	3.545075	4.244081	-0.062121
C	3.470884	0.356233	-0.514568
H	3.463518	-0.713652	-0.666875
C	4.628051	1.002800	-0.123501
H	5.529380	0.427989	0.064164
C	4.669606	2.417931	-0.004238
H	5.591073	2.902690	0.301026
H	1.636822	0.705447	-1.577475
H	3.052113	-3.546239	-0.279316
C	2.232954	-2.839559	-0.196359
C	1.977352	-2.290919	1.054535
C	1.561612	-2.488924	-1.360848
N	0.959882	-1.397803	1.340309
C	2.780731	-2.505091	2.240006
C	1.922183	-2.922251	-2.696440
N	0.490417	-1.612728	-1.429957
C	1.090824	-1.058814	2.674905
Fe	-0.515474	-0.819641	0.115799
C	2.251076	-1.725852	3.230784
H	3.637488	-3.161498	2.291506
C	1.070282	-2.301407	-3.565747

H	2.724955	-3.609033	-2.923339
C	0.148822	-1.513861	-2.768946
C	0.178438	-0.316335	3.415816
Cl	-1.517211	-2.845620	0.481153
N	-1.550500	-0.089275	1.678413
N	-2.034143	-0.352095	-1.087739
H	2.582861	-1.628657	4.254466
H	1.030393	-2.390305	-4.641812
C	-0.993454	-0.893735	-3.259524
C	-1.075167	0.077942	2.965972
H	0.413299	-0.137320	4.459815
C	-2.893167	0.238183	1.704533
C	-3.328579	-0.024598	-0.703282
C	-2.038565	-0.425591	-2.470425
H	-1.143191	-0.897142	-4.334018
C	-2.141862	0.575957	3.815029
C	-3.266261	0.652946	3.043362
C	-3.738438	0.224506	0.600744
C	-4.154958	0.130823	-1.879955
C	-3.355980	-0.090134	-2.967957
H	-2.035974	0.797650	4.867184
H	-4.259716	0.960040	3.336868
H	-4.780142	0.481694	0.760063
H	-5.205435	0.383176	-1.862977
H	-3.629113	-0.067063	-4.013054

3(D)

E=-1643.8961646au

N	-0.343783	1.014322	-0.554904
C	0.365544	2.130803	-0.779558
C	-0.460518	3.336041	-0.891819
C	-1.780235	2.927161	-0.747893
C	-1.736938	1.459264	-0.446545
C	1.783029	2.279357	-0.931873
C	0.121008	4.613698	-1.136208
H	-0.510767	5.492699	-1.216985
C	1.483137	4.703645	-1.275601
H	1.955985	5.660994	-1.466768
C	2.301403	3.527013	-1.178690
H	3.373906	3.633309	-1.310828
H	2.425096	1.418460	-0.877761
C	-3.027312	3.587656	-0.931000
H	-3.070094	4.669597	-1.003698
C	-2.919351	0.705114	-0.974918
H	-2.866840	-0.369780	-1.040126
C	-4.075995	1.381345	-1.213999
H	-4.968396	0.833887	-1.499965
C	-4.150006	2.823333	-1.139467
H	-5.105390	3.304674	-1.323092
H	-1.906799	1.389925	0.655579
C	-2.094476	-2.540004	-0.546933
N	-0.897913	-1.934062	-0.905064
C	-2.608623	-3.297682	-1.668382
C	-2.750359	-2.352682	0.662903
C	-0.639166	-2.313872	-2.210101
Fe	0.337334	-0.903252	0.287027
C	-1.725848	-3.137726	-2.700494
H	-3.527126	-3.866652	-1.656334
C	-2.322247	-1.487325	1.662444
H	-3.687970	-2.876214	0.816031
C	0.543146	-2.076082	-2.901702
N	-1.140907	-0.761450	1.634527
N	1.820157	-1.070650	-1.047326
N	1.587347	0.086913	1.497184
Cl	1.003944	-2.856095	1.241620
H	-1.775148	-3.560663	-3.693550
C	-3.062284	-1.163404	2.863062
C	1.703114	-1.562678	-2.335185
H	0.604172	-2.436339	-3.923216
C	-1.107670	-0.016156	2.803316
C	3.173627	-0.866585	-0.824860
C	2.967068	0.160244	1.397411
C	1.243872	0.717071	2.680516
C	-2.326619	-0.240517	3.554368
H	-4.018060	-1.590886	3.129715
C	3.013072	-1.617800	-2.955234
C	-0.021679	0.726201	3.254714
C	3.920135	-1.213944	-2.016638

C	3.717028	-0.322597	0.332091
C	3.499662	0.879845	2.535722
C	2.437147	1.244373	3.313590
H	-2.558423	0.224442	4.501786
H	3.200417	-1.957321	-3.963723
H	-0.137812	1.256778	4.193962
H	4.994378	-1.146094	-2.110087
H	4.794987	-0.213154	0.381740
H	4.548912	1.077122	2.701364
H	2.446949	1.789212	4.246573

$TS_{34(D)}$

E=-1643.8776493au

N	-0.352106	1.135521	-0.449526
C	0.384710	2.304120	-0.572798
C	-0.436248	3.475412	-0.702457
C	-1.789367	3.049143	-0.629612
C	-1.758782	1.610138	-0.458253
C	1.792769	2.440615	-0.597243
C	0.144381	4.754145	-0.856124
H	-0.484113	5.633996	-0.951773
C	1.523331	4.859754	-0.891966
H	1.992510	5.830124	-1.017677
C	2.336996	3.702419	-0.768948
H	3.416215	3.810280	-0.812141
H	2.428720	1.576715	-0.514284
C	-3.021044	3.724116	-0.753106
H	-3.045038	4.805123	-0.845516
C	-2.973170	0.861026	-0.639671
H	-2.961101	-0.215938	-0.626878
C	-4.155644	1.561569	-0.765781
H	-5.086370	1.010638	-0.855275
C	-4.190456	2.983494	-0.805169
H	-5.146012	3.486667	-0.909720
H	-1.288357	1.330048	0.628065
H	-3.674089	-3.006262	0.463247
C	-2.741781	-2.458195	0.380858
C	-2.089247	-2.469599	-0.845507
C	-2.319417	-1.729325	1.485329
N	-0.888359	-1.827331	-1.113171
C	-2.602786	-3.065924	-2.060258
C	-3.059034	-1.573494	2.717841
N	-1.149563	-0.983302	1.545872
C	-0.627150	-2.028615	-2.457883
Fe	0.347181	-0.983737	0.211758
C	-1.716313	-2.772038	-3.058294
H	-3.524987	-3.624610	-2.128257
C	-2.338167	-0.731562	3.519035
H	-4.007070	-2.046652	2.928973
C	-1.125852	-0.394309	2.803439
C	0.557597	-1.704718	-3.106839
Cl	1.004827	-3.026361	0.915639
N	1.823731	-0.948887	-1.130485
N	1.574519	-0.126760	1.536321
H	-1.765396	-3.053551	-4.100198
H	-2.576203	-0.391810	4.516600
C	-0.046520	0.291126	3.349580
C	1.713401	-1.266310	-2.473431
H	0.622099	-1.924495	-4.167144
C	3.174699	-0.756089	-0.881827
C	2.955553	-0.032412	1.454499
C	1.222375	0.354266	2.786326
H	-0.170108	0.701681	4.346074
C	3.023226	-1.222073	-3.092168
C	3.925014	-0.933130	-2.106922
C	3.711547	-0.365140	0.338102
C	3.477648	0.543718	2.675119
C	2.408921	0.805794	3.485290
H	3.214714	-1.420440	-4.136763
H	4.997901	-0.836952	-2.189313
H	4.788122	-0.251460	0.403909
H	4.524603	0.726312	2.869129
H	2.410504	1.233654	4.477345

4(D)

E=-1126.5993569au

N	-1.475621	-1.342324	-0.238720
C	-2.844635	-1.095668	-0.293231

C	-3.578260	-2.339505	-0.273098
C	-2.658306	-3.344732	-0.185363
C	-1.352839	-2.727170	-0.163081
N	1.346952	-1.470711	-0.238415
C	1.097032	-2.838556	-0.162225
C	2.340175	-3.573322	-0.183926
C	3.348790	-2.656995	-0.271477
C	2.732788	-1.351076	-0.292368
N	1.475724	1.342220	-0.238806
C	2.844740	1.095544	-0.293031
C	3.578296	2.339431	-0.275390
C	2.658631	3.344547	-0.183037
C	1.352978	2.727151	-0.163586
N	-1.346987	1.470716	-0.238836
C	-1.097099	2.838655	-0.162823
C	-2.340318	3.573436	-0.184450
C	-3.348956	2.657012	-0.271618
C	-2.732877	1.351079	-0.292852
C	3.430939	-0.157200	-0.331365
C	0.157081	3.421063	-0.112678
H	0.206314	4.503193	-0.056515
C	-0.157009	-3.420979	-0.112078
H	-0.206219	-4.503066	-0.056412
C	-3.430939	0.157074	-0.331693
H	-4.513637	0.206594	-0.369140
Fe	0.000007	0.000002	-0.029401
H	4.513579	-0.206776	-0.369313
H	-2.831618	-4.410148	-0.144356
H	-4.654846	-2.416046	-0.315251
H	-4.413952	2.832512	-0.312537
H	-2.414647	4.650319	-0.142695
H	2.832058	4.409915	-0.140232
H	4.654798	2.416003	-0.319133
H	4.413732	-2.832546	-0.312717
H	2.414501	-4.650157	-0.142196
Cl	-0.000118	0.000123	2.197918

$TS_{24(D)}$

E=-1643.8402994au

C	2.227567	4.023245	0.000015
H	3.215121	4.470358	0.000018
C	1.110300	4.866548	0.000018
H	1.249678	5.942361	0.000024
C	-0.191416	4.322268	0.000013
H	-1.053691	4.980441	0.000015
C	-0.374141	2.954593	0.000006
H	-1.363599	2.525098	-0.000002
C	0.751468	2.052737	0.000003
N	0.563626	0.739292	-0.000001
C	2.103466	2.632502	0.000009
C	3.256475	1.721990	0.000007
C	3.017546	0.344058	0.000002
H	1.656252	0.207567	0.000013
C	4.610443	2.134206	0.000004
H	4.864957	3.188926	0.000006
C	4.009048	-0.620523	-0.000013
H	3.766301	-1.677642	-0.000021
C	5.346159	-0.184990	-0.000015
H	6.152070	-0.912535	-0.000024
C	5.635368	1.186667	-0.000006
H	6.668474	1.518970	-0.000008
H	-4.511233	2.046793	2.644532
C	-3.620360	1.450079	2.511301
C	-2.761087	0.986926	3.467289
C	-3.119659	0.996591	1.230788
C	-1.739740	0.219088	2.787479
H	-2.815079	1.121923	4.537834
N	-1.962819	0.254904	1.417214
C	-3.675619	1.320705	0.000282
C	-0.758479	-0.524149	3.425408
C	-3.119832	0.996703	-1.230331
H	-4.586992	1.908945	0.000375
C	0.084168	-1.428381	2.792043
H	-0.706167	-0.461532	4.507093
N	-1.963001	0.255059	-1.416978
C	-3.620711	1.450304	-2.510735

N	0.142707	-1.640950	1.426691
C	0.957495	-2.362148	3.471360
C	-1.740097	0.219384	-2.787274
C	-2.761551	0.987264	-3.466879
H	-4.511614	2.047013	-2.643792
C	1.010467	-2.703321	1.232368
C	1.514073	-3.159981	2.511466
H	1.096952	-2.405236	4.541772
C	-0.758886	-0.523753	-3.425399
H	-2.815684	1.122365	-4.537403
C	1.393503	-3.216517	-0.000278
H	2.205211	-3.980302	2.641517
C	0.083864	-1.428029	-2.792234
H	-0.706704	-0.461016	-4.507083
C	1.010355	-2.703147	-1.232818
H	2.074592	-4.061324	-0.000369
N	0.142560	-1.640763	-1.426914
C	0.957136	-2.361692	-3.471761
C	1.513833	-3.159635	-2.512027
H	1.096478	-2.404644	-4.542194
H	2.204972	-3.979927	-2.642256
Fe	-0.941490	-0.714541	0.000005
Cl	-2.427647	-2.404052	-0.000048

1(Q)

E=-1753.4050468au

N	-1.077368	0.520624	-1.244848
C	-1.927559	1.661320	-1.084779
C	-3.313865	1.601239	-0.797093
C	-4.041693	0.325763	-0.539142
C	-3.566225	-0.597552	0.412410
H	-2.639230	-0.392485	0.940834
N	-1.500239	-0.493976	-1.814365
N	-1.710500	-1.490888	-2.322872
C	-1.277232	2.899660	-1.202952
H	-0.212180	2.903988	-1.403161
C	-4.013682	2.820375	-0.705775
H	-5.074726	2.787477	-0.479743
C	-1.993392	4.090692	-1.086487
C	-3.372611	4.052117	-0.851515
H	-1.479208	5.040897	-1.186375
H	-3.940913	4.972202	-0.763568
C	-5.256019	0.049098	-1.196344
H	-5.628825	0.747397	-1.939578
C	-4.282049	-1.765247	0.690928
H	-3.895986	-2.463980	1.426637
C	-5.486569	-2.029403	0.028482
C	-5.972359	-1.117676	-0.915418
H	-6.040653	-2.937595	0.244015
H	-6.903082	-1.317337	-1.437208
H	0.185197	-4.606616	-0.067402
C	0.481698	-3.567636	0.020689
C	1.230331	-3.022525	-1.007219
C	0.067578	-2.872008	1.143448
N	1.697880	-1.712726	-1.061117
C	1.628823	-3.738250	-2.195495
C	-0.744557	-3.432151	2.196592
N	0.351341	-1.538356	1.419971
C	2.389872	-1.609857	-2.263523
C	2.340675	-2.867253	-2.970664
H	1.383217	-4.770144	-2.398630
C	-0.955476	-2.440525	3.114234
H	-1.097484	-4.452797	2.218695
C	-0.270000	-1.264194	2.634220
C	3.043924	-0.480010	-2.722723
H	2.796575	-3.045398	-3.933459
H	-1.513657	-2.488952	4.037758
C	-0.239211	-0.049407	3.297837
C	3.106172	0.722797	-2.041266
H	3.548311	-0.543735	-3.680300
C	0.429922	1.074901	2.846616
H	-0.770056	0.024057	4.240367
N	2.525922	0.982992	-0.804584
C	3.796677	1.897008	-2.519381
N	1.165881	1.161975	1.669157
C	0.471057	2.335401	3.548996
C	2.851697	2.301623	-0.504876
C	3.642571	2.869011	-1.571442

H	4.327766	1.954289	-3.458176
C	1.671900	2.457225	1.636874
C	1.238775	3.186117	2.805143
H	-0.025551	2.528114	4.488676
C	2.464661	2.987254	0.633743
H	4.022153	3.880318	-1.579987
H	1.495412	4.214242	3.014409
H	2.795404	4.014245	0.741617
Fe	1.648564	-0.351590	0.428010
Cl	3.574789	-1.045989	1.526602

$TS_{12(Q)}$

E=-1753.3497117au

N	-1.085339	0.517200	-1.045475
C	-1.988139	1.548164	-1.034657
C	-3.402078	1.424267	-0.787789
C	-4.066497	0.108328	-0.608490
C	-3.523075	-0.876338	0.243670
H	-2.578436	-0.685900	0.741457
N	-1.563498	-0.733403	-2.118811
N	-1.249645	-1.780316	-2.356431
C	-1.428491	2.849088	-1.187853
H	-0.367941	2.913119	-1.401213
C	-4.168010	2.597785	-0.727273
H	-5.233294	2.516020	-0.537044
C	-2.208678	3.993366	-1.057079
C	-3.588015	3.867299	-0.843654
H	-1.756045	4.974987	-1.152648
H	-4.211689	4.751944	-0.763853
C	-4.193130	-2.083909	0.452346
H	-3.757584	-2.827018	1.113433
C	-5.295576	-0.160882	-1.245515
H	-5.717468	0.577753	-1.920085
C	-5.412749	-2.337364	-0.188103
C	-5.961612	-1.371535	-1.039244
H	-6.902097	-1.562701	-1.546450
H	-5.928322	-3.279241	-0.028460
H	4.169606	2.934327	-2.880498
C	3.583456	2.673416	-2.011512
C	3.089609	1.346796	-1.726582
C	3.173602	3.483822	-0.990261
N	2.372278	1.353135	-0.536008
C	3.316415	0.238945	-2.524505
C	2.418202	2.663153	-0.072820
H	3.357120	4.540068	-0.857624
Fe	1.646768	-0.248541	0.451074
C	2.863642	-1.038397	-2.243041
H	3.900156	0.378965	-3.427439
C	1.809596	3.131032	1.079508
Cl	3.566055	-0.688742	1.698071
N	0.536259	-1.763238	1.189019
N	2.109552	-1.404541	-1.133724
N	0.785920	0.998041	1.780212
C	3.128589	-2.196460	-3.063620
C	1.039828	2.356769	1.930259
H	1.930603	4.180533	1.323772
C	-0.240064	-1.743550	2.342054
C	0.548828	-3.086842	0.763465
C	1.912091	-2.776901	-1.247943
C	-0.030154	0.645853	2.849668
C	2.546332	-3.268123	-2.448031
H	3.691581	-2.176927	-3.985234
C	0.366247	2.857586	3.104990
C	-0.724913	-3.072688	2.632664
C	-0.510320	-0.625315	3.113000
C	-0.235139	-3.900936	1.661494
C	1.198875	-3.564407	-0.361416
C	-0.296448	1.804479	3.669103
H	2.534675	-4.299980	-2.766974
H	0.403106	3.883726	3.440264
H	-1.347476	-3.325525	3.478583
H	-1.133050	-0.756698	3.990864
H	-0.382123	-4.965343	1.550927
H	1.126572	-4.624987	-0.574223
H	-0.908840	1.796411	4.558842

2(Q)

E=-1643. 8771065au

N	0. 348860	0. 812881	−0. 248294
C	0. 646925	2. 073467	−0. 521865
C	2. 027930	2. 526386	−0. 608276
C	3. 167334	1. 591020	−0. 461753
C	3. 145958	0. 305276	−1. 038932
H	2. 272975	−0. 023319	−1. 593029
C	−0. 414420	3. 030422	−0. 708552
C	2. 254074	3. 888656	−0. 837849
H	3. 278356	4. 235452	−0. 922510
C	1. 206267	4. 802860	−1. 000411
H	1. 428237	5. 847930	−1. 188295
C	−0. 129844	4. 363850	−0. 940264
H	−0. 941740	5. 070627	−1. 075804
H	−1. 433920	2. 674246	−0. 653409
C	4. 327384	1. 993934	0. 234017
H	4. 351992	2. 968031	0. 712036
C	4. 251069	−0. 543311	−0. 928095
H	4. 211572	−1. 527114	−1. 384025
C	5. 394580	−0. 129343	−0. 236070
H	6. 250408	−0. 791336	−0. 149115
C	5. 427910	1. 142946	0. 347487
H	6. 305467	1. 468305	0. 897185
C	1. 931132	−3. 664938	−0. 999285
C	1. 386989	−3. 397826	−2. 224582
C	1. 273030	−2. 797642	−0. 043160
H	2. 703484	−4. 378318	−0. 750011
C	0. 378645	−2. 377687	−2. 025012
H	1. 623344	−3. 850019	−3. 176873
N	0. 324731	−2. 024304	−0. 690050
C	1. 595588	−2. 719555	1. 303151
C	−0. 434411	−1. 855965	−3. 022598
Fe	−0. 957132	−0. 735284	0. 189033
C	1. 022152	−1. 844766	2. 214363
H	2. 374505	−3. 379504	1. 669707
C	−1. 471395	−0. 964161	−2. 807410
H	−0. 283809	−2. 215318	−4. 034849
Cl	−2. 336808	−2. 417666	0. 705097
N	0. 011155	−0. 937071	1. 943445
N	−2. 193876	0. 603609	1. 049303
N	−1. 828758	−0. 411971	−1. 578855
C	1. 411427	−1. 740353	3. 604224
C	−2. 405970	−0. 537752	−3. 823422
C	−0. 247930	−0. 278011	3. 132000
C	−2. 170110	1. 045504	2. 367211
C	−3. 316829	1. 175348	0. 472117
C	−2. 986732	0. 320178	−1. 809572
C	0. 634607	−0. 767304	4. 167886
H	2. 178778	−2. 340013	4. 071997
C	−3. 343431	0. 243537	−3. 208600
H	−2. 351309	−0. 824563	−4. 863559
C	−1. 247268	0. 666242	3. 326616
C	−3. 294453	1. 923889	2. 609009
C	−4. 006069	1. 996724	1. 445749
C	−3. 692173	1. 039901	−0. 856698
H	0. 636489	−0. 415300	5. 189202
H	−4. 204385	0. 726512	−3. 647743
H	−1. 346722	1. 095074	4. 317909
H	−3. 505205	2. 401837	3. 554693
H	−4. 912596	2. 550431	1. 248176
H	−4. 591318	1. 552894	−1. 180585

$TS_{23(Q)}$

E=-1643.8414045au

N	0. 305359	0. 880885	−0. 639360
C	−0. 191608	2. 122554	−0. 902959
C	0. 773490	3. 098023	−1. 354697
C	2. 101945	2. 490844	−1. 348888
C	2. 003949	1. 048845	−1. 535307
C	−1. 544452	2. 534372	−0. 762634
C	0. 400489	4. 407841	−1. 626276
H	1. 141567	5. 130445	−1. 953525
C	−0. 946205	4. 785428	−1. 488891
H	−1. 247594	5. 803361	−1. 712843
C	−1. 901890	3. 847860	−1. 063511
H	−2. 939327	4. 149208	−0. 960897
H	−2. 289526	1. 830663	−0. 432402

C	3.270041	3.080005	-0.889436
H	3.295539	4.149018	-0.700156
C	3.158226	0.267904	-1.171604
H	3.140760	-0.800255	-1.336951
C	4.308491	0.882584	-0.693829
H	5.170820	0.275003	-0.438103
C	4.391061	2.283891	-0.580270
H	5.302854	2.748791	-0.220990
H	1.472329	0.696949	-2.421469
H	3.219473	-3.408837	0.218085
C	2.366182	-2.738549	0.216295
C	2.249948	-1.842984	1.271590
C	1.520826	-2.778461	-0.886741
N	1.222175	-0.930559	1.437560
C	3.235486	-1.655968	2.317781
C	1.744370	-3.569602	-2.079486
N	0.386121	-2.000935	-1.054077
C	1.528112	-0.189014	2.562065
Fe	-0.457460	-0.845492	0.352653
C	2.805043	-0.618281	3.096436
H	4.136415	-2.242975	2.424720
C	0.749301	-3.256639	-2.964543
H	2.561164	-4.264701	-2.211438
C	-0.120160	-2.304207	-2.305664
C	0.673783	0.722441	3.172914
Cl	-1.221214	-2.698002	1.400250
N	-1.287197	0.316650	1.735021
N	-2.130236	-0.768303	-0.734972
H	3.278210	-0.197333	3.971735
H	0.586389	-3.654806	-3.955619
C	-1.353651	-1.884110	-2.791489
C	-0.657721	0.902012	2.824449
H	1.034568	1.234628	4.058493
C	-2.639192	0.593078	1.864407
C	-3.375966	-0.364724	-0.280767
C	-2.313258	-1.231693	-2.029521
H	-1.635426	-2.201522	-3.789831
C	-1.636424	1.602326	3.629280
C	-2.857928	1.390864	3.052978
C	-3.621796	0.237538	0.947749
C	-4.359998	-0.561706	-1.325605
C	-3.701554	-1.070545	-2.409991
H	-1.409372	2.150082	4.532399
H	-3.823683	1.742300	3.386594
H	-4.646127	0.510292	1.178036
H	-5.410941	-0.329239	-1.230607
H	-4.110671	-1.347968	-3.370689

3(Q)

E= -1643.9016764au

N	-1.456356	0.182043	-1.012021
C	-2.194923	1.281183	-1.024561
C	-3.634587	1.051394	-0.812623
C	-3.783673	-0.322717	-0.663907
C	-2.385369	-0.884050	-0.677892
C	-1.732412	2.628411	-1.232264
C	-4.547418	2.148420	-0.821766
H	-5.609229	1.980648	-0.667553
C	-4.058565	3.413677	-1.034809
H	-4.733124	4.263775	-1.049833
C	-2.649733	3.645919	-1.242302
H	-2.317469	4.666330	-1.408963
H	-0.675774	2.807907	-1.386940
C	-4.899174	-1.208288	-0.610920
H	-5.904020	-0.822271	-0.467122
C	-2.274891	-2.275956	-1.215502
H	-1.296064	-2.652747	-1.489154
C	-3.384250	-3.062988	-1.211507
H	-3.310459	-4.104975	-1.507735
C	-4.692456	-2.543975	-0.860120
H	-5.534976	-3.228640	-0.861138
H	-2.135303	-1.034404	0.402537
H	-0.259177	-3.817692	2.444365
C	0.073881	-2.926555	1.924232
C	0.688939	-3.090901	0.694134
C	-0.165701	-1.702091	2.525450
N	1.169859	-2.065736	-0.112649
C	0.880445	-4.362870	0.038805

C	-0.852077	-1.526840	3.783841
N	0.200942	-0.462699	2.009394
C	1.660195	-2.680831	-1.258533
Fe	1.367202	-0.125160	0.395652
C	1.472577	-4.109896	-1.167613
H	0.592271	-5.316306	0.456896
C	-0.897771	-0.184006	4.034466
H	-1.241182	-2.334683	4.386199
C	-0.232909	0.477647	2.936562
C	2.255243	-2.034435	-2.329304
Cl	3.414488	-0.378122	1.501156
N	2.144177	0.256672	-1.421583
N	1.212702	1.855390	0.722004
H	1.768663	-4.815711	-1.929900
H	-1.329872	0.324661	4.883810
C	-0.032708	1.845499	2.852134
C	2.480669	-0.670649	-2.398946
H	2.585375	-2.642668	-3.164074
C	2.590353	1.484137	-1.892350
C	1.808898	2.865344	-0.022974
C	0.650669	2.479602	1.828626
H	-0.420561	2.461395	3.655869
C	3.137165	-0.007177	-3.502191
C	3.210468	1.319801	-3.187163
C	2.455830	2.696337	-1.235952
C	1.617281	4.138592	0.632363
C	0.898447	3.901501	1.769867
H	3.494871	-0.506321	-4.390814
H	3.638175	2.124232	-3.767431
H	2.869486	3.577192	-1.714232
H	1.987030	5.081691	0.257119
H	0.563846	4.611684	2.511805

$TS_{34(Q)}$

E=-1643.8893812au

N	-1.461352	0.084684	-1.611567
C	-2.243089	1.191398	-1.429588
C	-3.607809	0.889701	-1.072504
C	-3.692932	-0.525411	-0.971428
C	-2.351279	-1.019779	-1.262129
C	-1.822045	2.538845	-1.571577
C	-4.537270	1.940782	-0.884998
H	-5.567962	1.726810	-0.618393
C	-4.109149	3.246154	-1.053244
H	-4.808965	4.065404	-0.920635
C	-2.757060	3.541463	-1.396551
H	-2.461924	4.579067	-1.517920
H	-0.790901	2.756013	-1.824932
C	-4.739205	-1.443730	-0.734239
H	-5.734718	-1.090853	-0.482568
C	-2.153484	-2.427032	-1.524091
H	-1.181679	-2.786414	-1.843386
C	-3.208551	-3.280057	-1.286255
H	-3.073436	-4.347896	-1.428403
C	-4.490396	-2.799043	-0.878532
H	-5.288864	-3.514428	-0.709952
H	-1.597172	-0.718889	-0.374697
H	-0.379505	-3.959953	1.995270
C	-0.013379	-3.021958	1.593626
C	0.886902	-3.077573	0.543435
C	-0.499357	-1.850777	2.147333
N	1.462617	-1.979288	-0.088511
C	1.335316	-4.297777	-0.082983
C	-1.469361	-1.788048	3.211723
N	-0.140876	-0.561393	1.752642
C	2.266742	-2.502637	-1.095832
Fe	1.386512	-0.059612	0.524282
C	2.180238	-3.943267	-1.097569
H	1.032591	-5.288840	0.221886
C	-1.697196	-0.465748	3.474344
H	-1.912404	-2.651129	3.686441
C	-0.862670	0.297576	2.580100
C	3.052483	-1.765275	-1.964530
Cl	3.098821	-0.189476	2.087462
N	2.506481	0.466087	-1.064110
N	0.935600	1.883306	0.809372
H	2.707942	-4.586679	-1.786276
H	-2.361142	-0.033670	4.208567

C	-0.774885	1.678726	2.577090
C	3.162957	-0.386396	-1.944730
H	3.630186	-2.306929	-2.705075
C	2.928992	1.748318	-1.395401
C	1.577861	2.976068	0.237631
C	0.065308	2.411015	1.757058
H	-1.398280	2.224397	3.276352
C	4.000123	0.377397	-2.839555
C	3.859509	1.692468	-2.498062
C	2.513057	2.916803	-0.781023
C	1.102805	4.198984	0.840572
C	0.167527	3.850820	1.773406
H	4.611474	-0.051250	-3.620022
H	4.331405	2.555494	-2.944323
H	2.934262	3.850992	-1.135196
H	1.446276	5.187078	0.571406
H	-0.407951	4.496867	2.419896

4(Q)

E=-1126.6137346au

N	-1.414288	1.411986	-0.244591
C	-1.226451	2.791127	-0.251361
C	-2.502790	3.464072	-0.269350
C	-3.468125	2.497182	-0.269326
C	-2.793126	1.221929	-0.251376
N	-1.411991	-1.414278	-0.244626
C	-2.791132	-1.226447	-0.251402
C	-3.464070	-2.502789	-0.269483
C	-2.497177	-3.468120	-0.269338
C	-1.221926	-2.793114	-0.251435
N	1.414290	-1.411980	-0.244617
C	1.226452	-2.791120	-0.251423
C	2.502792	-3.464065	-0.269403
C	3.468126	-2.497175	-0.269384
C	2.793128	-1.221922	-0.251388
N	1.411992	1.414284	-0.244582
C	2.791134	1.226454	-0.251354
C	3.464072	2.502795	-0.269403
C	2.497178	3.468127	-0.269238
C	1.221927	2.793121	-0.251358
C	0.002787	-3.436518	-0.248537
C	3.436534	0.002789	-0.248466
H	4.520706	0.003675	-0.250900
C	-3.436532	-0.002783	-0.248487
H	-4.520704	-0.003669	-0.250924
C	-0.002785	3.436524	-0.248452
H	-0.003671	4.520696	-0.250854
Fe	0.000000	-0.000001	0.040185
H	0.003673	-4.520690	-0.250962
H	-4.541092	2.620717	-0.280892
H	-2.628051	4.536839	-0.280933
H	2.620709	4.541095	-0.280747
H	4.536837	2.628061	-0.281037
H	4.541094	-2.620710	-0.280959
H	2.628053	-4.536832	-0.280999
H	-2.620707	-4.541088	-0.280874
H	-4.536836	-2.628054	-0.281124
Cl	-0.000008	-0.000030	2.353830

$TS_{25(Q)}$

E= -1643.8469245au

C	2.194215	4.029711	-0.000639
H	3.179026	4.482496	-0.000729
C	1.072591	4.864652	-0.000718
H	1.204824	5.941438	-0.000867
C	-0.223855	4.312095	-0.000599
H	-1.091375	4.963235	-0.000650
C	-0.395389	2.940841	-0.000418
H	-1.382200	2.505496	-0.000310
C	0.733902	2.052924	-0.000349
N	0.552930	0.728354	-0.000243
C	2.077153	2.635947	-0.000452
C	3.238572	1.735759	-0.000381
C	3.020796	0.355306	-0.000197
H	1.612459	0.211995	-0.000153
C	4.589407	2.161814	-0.000496
H	4.832305	3.219157	-0.000645
C	4.020500	-0.600731	-0.000119

H	3.788655	-1.660113	0.000027
C	5.351838	-0.149585	-0.000236
H	6.166315	-0.867486	-0.000183
C	5.624561	1.226216	-0.000424
H	6.653755	1.570394	-0.000516
H	-4.529493	2.012987	2.644187
C	-3.633599	1.423798	2.511155
C	-2.771905	0.965896	3.467465
C	-3.127656	0.976531	1.230527
C	-1.743304	0.207776	2.787653
H	-2.828392	1.098432	4.538185
N	-1.964838	0.244527	1.417309
C	-3.685947	1.296701	0.000094
C	-0.756974	-0.528378	3.426180
C	-3.127926	0.976112	-1.230355
H	-4.602117	1.877396	0.000094
C	0.093670	-1.425025	2.792998
H	-0.706955	-0.466846	4.508010
N	-1.965147	0.244048	-1.417143
C	-3.634139	1.422963	-2.511020
N	0.157008	-1.634985	1.427318
C	0.973002	-2.353116	3.472325
C	-1.743898	0.206861	-2.787519
C	-2.772646	0.964753	-3.467362
H	-4.530067	2.012101	-2.644055
C	1.032953	-2.690525	1.232804
C	1.537630	-3.145013	2.512277
H	1.110564	-2.396920	4.542949
C	-0.757698	-0.529489	-3.426016
H	-2.829357	1.096938	-4.538113
C	1.420500	-3.200552	0.000286
H	2.234618	-3.960357	2.642408
C	0.093083	-1.425924	-2.792719
H	-0.707905	-0.468307	-4.507876
C	1.032692	-2.690915	-1.232310
H	2.107852	-4.040254	0.000345
N	0.156687	-1.635455	-1.426986
C	0.972292	-2.354220	-3.471926
C	1.537118	-3.145806	-2.511738
H	1.109639	-2.398365	-4.542562
H	2.234090	-3.961184	-2.641745
Fe	-0.930309	-0.711853	0.000132
Cl	-2.402584	-2.411397	0.000609

5(Q)

E=-1643.8508629au

C	-2.370240	3.853204	-0.125846
H	-3.375292	4.252821	-0.199007
C	-1.289541	4.741113	-0.131436
H	-1.471433	5.809086	-0.188905
C	0.028346	4.248094	-0.077800
H	0.867319	4.935473	-0.083891
C	0.255086	2.885698	-0.030536
H	1.259165	2.492905	0.002096
C	-0.829123	1.945778	-0.030250
N	-0.555224	0.633772	0.009753
C	-2.194242	2.464532	-0.065867
C	-3.371569	1.571507	-0.035989
C	-3.349658	0.258158	-0.496042
H	-1.406260	0.061386	-0.000693
C	-4.630795	1.995570	0.470867
H	-4.726623	2.990666	0.893047
C	-4.407356	-0.625394	-0.533461
H	-4.296899	-1.632560	-0.921159
C	-5.639551	-0.161306	-0.039554
H	-6.505106	-0.816511	-0.038038
C	-5.736789	1.144821	0.461895
H	-6.682191	1.498363	0.860083
H	4.433801	2.130488	-2.769716
C	3.570831	1.501202	-2.606272
C	2.729056	0.958904	-3.535302
C	3.099879	1.076709	-1.304264
C	1.745661	0.177491	-2.815443
H	2.769941	1.050056	-4.611013
N	1.975429	0.280084	-1.450928
C	3.666828	1.456310	-0.095030
C	0.785442	-0.621451	-3.416706
C	3.165145	1.124697	1.156464

H	4.552479	2.081540	-0.131580
C	-0.041392	-1.509378	-2.742275
H	0.727290	-0.605815	-4.499709
N	2.043997	0.343517	1.391158
C	3.702831	1.598087	2.414953
N	-0.094766	-1.664946	-1.368219
C	-0.925682	-2.463063	-3.377094
C	1.881913	0.299523	2.768521
C	2.904837	1.101541	3.406232
H	4.576258	2.227011	2.510923
C	-0.976971	-2.706096	-1.124943
C	-1.492722	-3.208718	-2.381685
H	-1.067590	-2.552172	-4.444385
C	0.946069	-0.464945	3.449040
H	2.999970	1.237592	4.473837
C	-1.351778	-3.172164	0.128330
H	-2.190938	-4.028290	-2.474061
C	0.085570	-1.377230	2.854034
H	0.938097	-0.399751	4.531846
C	-0.922567	-2.646219	1.339540
H	-2.054012	-3.998366	0.164268
N	-0.029566	-1.597480	1.492791
C	-0.771968	-2.295957	3.572635
C	-1.382939	-3.086230	2.640384
H	-0.867832	-2.332225	4.648130
H	-2.082824	-3.893291	2.802370
Fe	0.997035	-0.670719	0.016618
Cl	2.529706	-2.319004	0.019941

1(S)

E=-1753.4013337au

N	-1.225205	0.638876	-1.313075
C	-2.119702	1.720070	-1.047714
C	-3.480128	1.580395	-0.675240
C	-4.128311	0.261851	-0.421998
C	-3.554213	-0.666734	0.468101
H	-2.607078	-0.434071	0.947587
N	-1.627979	-0.398760	-1.852427
N	-1.809344	-1.406664	-2.351605
C	-1.539468	2.994478	-1.152805
H	-0.490501	3.058897	-1.417850
C	-4.229936	2.758147	-0.489751
H	-5.271492	2.662922	-0.199699
C	-2.302039	4.142483	-0.941858
C	-3.660027	4.025677	-0.623731
H	-1.841000	5.120436	-1.033107
H	-4.265098	4.911685	-0.462266
C	-5.364108	-0.053969	-1.018505
H	-5.812635	0.648530	-1.714416
C	-4.196408	-1.876692	0.746500
H	-3.735201	-2.578346	1.434685
C	-5.423655	-2.179086	0.144738
C	-6.006323	-1.263293	-0.738487
H	-5.920361	-3.119991	0.360151
H	-6.955150	-1.492305	-1.213606
H	0.099605	-4.561176	-0.130325
C	0.442897	-3.537032	-0.027485
C	1.145180	-2.997566	-1.100577
C	0.114799	-2.876781	1.153223
N	1.660872	-1.708116	-1.155472
C	1.436279	-3.685108	-2.340793
C	-0.656866	-3.440019	2.240759
N	0.460290	-1.567624	1.462933
C	2.261662	-1.572931	-2.400858
C	2.121616	-2.810369	-3.139251
H	1.141541	-4.699913	-2.564970
C	-0.778596	-2.468649	3.198979
H	-1.048845	-4.446733	2.259849
C	-0.081661	-1.296213	2.713039
C	2.886354	-0.422003	-2.871859
H	2.495533	-2.975632	-4.139275
H	-1.289394	-2.531400	4.148950
C	0.015287	-0.080348	3.384239
C	2.999410	0.787567	-2.192817
H	3.310289	-0.466756	-3.869758
C	0.650407	1.066472	2.917494
H	-0.462594	-0.016409	4.356307
N	2.525977	1.035375	-0.911415

C	3.611343	1.989430	-2.719931
N	1.317340	1.178029	1.704084
C	0.704861	2.334133	3.614486
C	2.816703	2.363270	-0.628131
C	3.499250	2.957355	-1.758800
H	4.059716	2.073024	-3.699299
C	1.780251	2.484827	1.623118
C	1.399210	3.205110	2.819750
H	0.262448	2.524043	4.581605
C	2.482217	3.024942	0.549653
H	3.839797	3.981723	-1.803327
H	1.632216	4.241883	3.014276
H	2.779609	4.065347	0.630886
Fe	1.880593	-0.402862	0.459991
Cl	3.823048	-1.100331	1.398338

$TS_{12(S)}$

E=-1753.3453316au

N	-1.201697	0.661712	-1.229037
C	-2.189132	1.597309	-1.083117
C	-3.559412	1.338499	-0.722525
C	-4.087872	-0.037976	-0.543970
C	-3.395661	-0.989336	0.235753
H	-2.434498	-0.727277	0.666424
N	-1.674089	-0.616331	-2.269609
N	-1.272079	-1.615743	-2.572199
C	-1.755834	2.949623	-1.209146
H	-0.725576	3.115740	-1.502857
C	-4.414219	2.435413	-0.539147
H	-5.448234	2.249687	-0.266373
C	-2.614878	4.012406	-0.951001
C	-3.956251	3.755763	-0.634857
H	-2.255861	5.033651	-1.027855
H	-4.643268	4.577140	-0.457994
C	-3.940792	-2.256211	0.458358
H	-3.396311	-2.968926	1.070121
C	-5.332384	-0.402153	-1.098009
H	-5.867523	0.312095	-1.716251
C	-5.177524	-2.603812	-0.099886
C	-5.871119	-1.672904	-0.881289
H	-6.826137	-1.936639	-1.324827
H	-5.595270	-3.591254	0.070498
H	4.125566	2.181287	-3.602217
C	3.604308	2.110889	-2.658589
C	3.086961	0.882782	-2.091547
C	3.298957	3.120966	-1.787321
N	2.478386	1.158434	-0.874997
C	3.168257	-0.373754	-2.684312
C	2.589703	2.527260	-0.672617
H	3.524417	4.173251	-1.883343
Fe	1.860461	-0.247654	0.536708
C	2.634749	-1.556283	-2.180376
H	3.680766	-0.434020	-3.638850
C	2.078064	3.222977	0.419139
Cl	3.777682	-0.653362	1.682339
N	0.504616	-1.505111	1.513292
N	1.946132	-1.679136	-0.981249
N	1.027266	1.334775	1.614797
C	2.698926	-2.848055	-2.831630
C	1.346786	2.678137	1.471167
H	2.249190	4.294387	0.443336
C	-0.171408	-1.216389	2.692004
C	0.337386	-2.862959	1.277470
C	1.573530	-3.012497	-0.869139
C	0.272858	1.225123	2.775788
C	2.048091	-3.742260	-2.026107
H	3.176398	-3.034363	-3.782632
C	0.783716	3.426311	2.575622
C	-0.772820	-2.427861	3.208671
C	-0.268827	0.044384	3.275083
C	-0.459206	-3.439782	2.340033
C	0.842080	-3.557278	0.181425
C	0.124232	2.534049	3.376721
H	1.891279	-4.797695	-2.194532
H	0.881626	4.493931	2.709171
H	-1.356034	-2.486995	4.116221
H	-0.834011	0.115756	4.198746
H	-0.734659	-4.482517	2.406115

H	0.628059	-4.619840	0.131644
H	-0.419837	2.734263	4.288407

2(S)

E=-1643.8834792au

N	0.936901	0.972475	-0.060892
C	1.679431	2.068583	-0.130056
C	3.134168	2.026610	-0.126262
C	3.869871	0.740272	-0.101780
C	3.405893	-0.391557	-0.804219
H	2.485050	-0.330984	-1.374727
C	1.016985	3.347714	-0.176491
C	3.821822	3.246273	-0.145323
H	4.906443	3.232321	-0.165893
C	3.154970	4.477528	-0.177934
H	3.728208	5.398305	-0.202740
C	1.747513	4.522305	-0.197306
H	1.234762	5.477997	-0.230332
H	-0.066752	3.355170	-0.187386
C	5.079273	0.628262	0.617213
H	5.439017	1.475376	1.192397
C	4.128813	-1.587227	-0.788581
H	3.751603	-2.442936	-1.339908
C	5.327238	-1.681178	-0.071899
H	5.885945	-2.611801	-0.059366
C	5.799359	-0.567602	0.632829
H	6.721096	-0.633171	1.202394
C	0.678583	-3.776512	-1.878254
C	0.259957	-3.092606	-2.985878
C	0.246276	-3.022769	-0.724253
H	1.224495	-4.707694	-1.831754
C	-0.437510	-1.916349	-2.520941
H	0.397665	-3.351579	-4.025584
N	-0.434926	-1.883048	-1.132057
C	0.497359	-3.385758	0.588579
C	-1.022403	-0.972658	-3.349518
Fe	-1.428317	-0.585153	0.051136
C	0.115420	-2.647425	1.695486
H	1.042736	-4.306942	0.761233
C	-1.701482	0.150162	-2.908344
H	-0.949231	-1.128512	-4.420176
Cl	-3.428472	-1.795833	0.131347
N	-0.590996	-1.451849	1.666154
N	-2.053270	0.938765	1.217573
N	-1.899171	0.507728	-1.579676
C	0.412252	-3.010417	3.061982
C	-2.317843	1.125458	-3.777149
C	-0.740350	-1.065638	2.991454
C	-2.009874	0.996758	2.605393
C	-2.771106	2.057787	0.812290
C	-2.633060	1.687232	-1.608839
C	-0.112734	-2.034209	3.860507
H	0.954451	-3.897388	3.355452
C	-2.893755	2.071312	-2.976576
H	-2.306235	1.077377	-4.856266
C	-1.398185	0.070336	3.432362
C	-2.707285	2.172828	3.070542
C	-3.178066	2.825502	1.966153
C	-3.046747	2.406915	-0.499693
H	-0.087523	-1.963349	4.938066
H	-3.446808	2.951458	-3.270519
H	-1.442959	0.243025	4.501887
H	-2.817213	2.448011	4.109304
H	-3.750261	3.740702	1.921556
H	-3.622703	3.309690	-0.670749

$TS_{23(S)}$

E=-1643.8470858au

N	1.630008	0.357806	-0.375542
C	2.432406	1.450119	-0.388702
C	3.848548	1.220048	-0.552837
C	4.069629	-0.230691	-0.598482
C	2.884500	-0.907334	-1.109455
C	1.962098	2.782175	-0.221235
C	4.744309	2.281127	-0.534352
H	5.810213	2.105392	-0.643604
C	4.255637	3.593170	-0.386486
H	4.949732	4.427378	-0.387342

C	2.877478	3.833306	-0.234371
H	2.522937	4.852512	-0.117221
H	0.901851	2.957615	-0.088601
C	5.047926	-0.934361	0.091290
H	5.890157	-0.401667	0.523687
C	2.747218	-2.308752	-0.820313
H	1.886914	-2.845543	-1.204697
C	3.735601	-2.980801	-0.110064
H	3.621873	-4.041826	0.091571
C	4.904274	-2.318403	0.313917
H	5.674687	-2.862940	0.849519
H	2.505584	-0.585119	-2.081213
H	-1.468084	-2.470239	-3.753059
C	-1.423622	-1.914490	-2.822985
C	-1.128275	-2.616930	-1.666712
C	-1.677305	-0.554748	-2.873264
N	-1.027335	-2.072110	-0.392388
C	-0.877953	-4.038677	-1.615529
C	-2.000397	0.170679	-4.079559
N	-1.677412	0.309949	-1.784815
C	-0.721340	-3.132556	0.451593
Fe	-1.491384	-0.190116	0.160202
C	-0.630759	-4.356807	-0.308789
H	-0.899631	-4.695326	-2.473091
C	-2.207099	1.473133	-3.722808
H	-2.062636	-0.273243	-5.062361
C	-2.007727	1.559880	-2.295036
C	-0.508482	-3.040684	1.816431
Cl	-3.760018	-0.592818	0.551413
N	-0.862075	-0.608379	2.027409
N	-1.534228	1.768668	0.638594
H	-0.407784	-5.325244	0.114784
H	-2.470773	2.308032	-4.355451
C	-2.126138	2.725722	-1.558212
C	-0.561261	-1.863312	2.541743
H	-0.271906	-3.953013	2.352484
C	-0.799400	0.266968	3.104215
C	-1.398180	2.320605	1.907606
C	-1.901916	2.819665	-0.195122
H	-2.403675	3.630610	-2.087292
C	-0.302005	-1.766384	3.959552
C	-0.445901	-0.453040	4.305659
C	-1.050108	1.627279	3.054106
C	-1.675950	3.736425	1.860906
C	-1.989434	4.043633	0.566033
H	-0.043324	-2.602590	4.592470
H	-0.330069	0.000782	5.278972
H	-0.975493	2.187988	3.979148
H	-1.637259	4.395805	2.715651
H	-2.257977	5.004227	0.151133

3(S)

E=-1643.8969609au

N	1.587848	-0.100636	-1.616916
C	2.571011	-0.953883	-1.382696
C	3.806245	-0.339944	-0.865913
C	3.542136	1.022846	-0.771723
C	2.087185	1.172710	-1.133228
C	2.537180	-2.378075	-1.589726
C	4.951210	-1.148478	-0.599486
H	5.865830	-0.699978	-0.222669
C	4.875912	-2.500208	-0.832139
H	5.735597	-3.134551	-0.640426
C	3.665049	-3.109892	-1.326382
H	3.660087	-4.184114	-1.486264
H	1.623578	-2.836515	-1.950750
C	4.329261	2.183278	-0.520502
H	5.342988	2.091529	-0.141625
C	1.714560	2.490209	-1.729327
H	0.750122	2.586030	-2.216572
C	2.533726	3.555602	-1.516359
H	2.239160	4.543105	-1.858663
C	3.823939	3.413238	-0.870484
H	4.424404	4.305009	-0.719029
H	1.558956	1.212065	-0.144915
H	-0.333559	4.017233	2.038812
C	-0.543977	3.031819	1.636486
C	-1.331274	2.973308	0.490024

C	0.018248	1.945923	2.301360
N	-1.710337	1.807227	-0.163918
C	-1.859316	4.117001	-0.222252
C	0.868733	2.025297	3.468950
N	-0.132658	0.613269	1.930193
C	-2.458575	2.194797	-1.268505
Fe	-1.569671	-0.134878	0.600174
C	-2.549748	3.639203	-1.303740
H	-1.712512	5.146299	0.071331
C	1.228443	0.746038	3.798488
H	1.151690	2.943632	3.962608
C	0.602483	-0.138466	2.839745
C	-3.025698	1.330485	-2.200962
Cl	-3.412562	-0.266166	1.917269
N	-2.275039	-0.814311	-1.237593
N	-0.696170	-2.010074	0.865233
H	-3.075617	4.204097	-2.059862
H	1.859725	0.422074	4.613164
C	0.721276	-1.525220	2.827117
C	-2.932267	-0.057578	-2.197344
H	-3.580914	1.783359	-3.016025
C	-2.393265	-2.141298	-1.624928
C	-1.040680	-3.169816	0.184812
C	0.133921	-2.391371	1.910240
H	1.339399	-1.971896	3.598992
C	-3.489444	-0.937242	-3.204220
C	-3.159033	-2.217361	-2.852163
C	-1.836359	-3.227477	-0.955915
C	-0.419076	-4.307872	0.830369
C	0.303010	-3.829431	1.889521
H	-4.050797	-0.607892	-4.066539
H	-3.398939	-3.133572	-3.372005
H	-2.018889	-4.210367	-1.378322
H	-0.522931	-5.332679	0.504299
H	0.903218	-4.388382	2.592652

$TS_{34(S)}$

E=-1643.8859419au

N	1.557392	-0.109843	-1.764715
C	2.510810	-1.044381	-1.476653
C	3.760979	-0.483930	-1.023039
C	3.572896	0.923441	-0.970033
C	2.191272	1.147710	-1.385050
C	2.360643	-2.450113	-1.599798
C	4.849820	-1.337817	-0.723809
H	5.796887	-0.928576	-0.384841
C	4.687261	-2.703678	-0.877432
H	5.513552	-3.373725	-0.660811
C	3.446865	-3.255490	-1.314538
H	3.360967	-4.332543	-1.420635
H	1.412093	-2.862077	-1.924700
C	4.406088	2.028445	-0.688569
H	5.425261	1.876306	-0.346206
C	1.758062	2.486296	-1.716142
H	0.764886	2.647445	-2.120123
C	2.611878	3.528604	-1.430899
H	2.291813	4.547968	-1.624001
C	3.922435	3.308435	-0.906055
H	4.556954	4.165713	-0.705056
H	1.432858	0.735080	-0.547340
H	0.286570	3.872328	2.029186
C	-0.072129	2.930936	1.626544
C	-1.056688	2.997682	0.645002
C	0.515543	1.769757	2.118391
N	-1.640091	1.902519	0.018608
C	-1.608560	4.216789	0.094622
C	1.565186	1.715314	3.111050
N	0.193434	0.476110	1.714475
C	-2.539601	2.409079	-0.911955
Fe	-1.536823	-0.083341	0.668227
C	-2.516342	3.855479	-0.864512
H	-1.328495	5.213381	0.403770
C	1.872605	0.395597	3.307877
H	2.007405	2.578878	3.586075
C	1.014034	-0.381690	2.442151
C	-3.337040	1.645702	-1.759686
Cl	-3.102440	-0.143632	2.306026
N	-2.612554	-0.602090	-1.040461

N	-0.792161	-2.032524	0.680406
H	-3.119842	4.501047	-1.486029
H	2.611785	-0.022156	3.975804
C	1.003743	-1.770395	2.354359
C	-3.366418	0.256591	-1.829476
H	-3.989806	2.185516	-2.437945
C	-2.920955	-1.892768	-1.448854
C	-1.359011	-3.123386	0.035139
C	0.179535	-2.535476	1.535271
H	1.712582	-2.306442	2.976712
C	-4.175836	-0.518864	-2.745998
C	-3.903451	-1.839028	-2.511091
C	-2.352312	-3.055217	-0.937279
C	-0.733713	-4.340563	0.509474
C	0.212034	-3.979012	1.429986
H	-4.854927	-0.098770	-3.473623
H	-4.317277	-2.702934	-3.010579
H	-2.696822	-3.995671	-1.354844
H	-0.987776	-5.334753	0.171448
H	0.880280	-4.620912	1.985217

4(S)

E=-1126.6112127au

H	-3.095529	3.308332	-0.326483
C	-2.354603	2.516378	-0.290495
C	-2.829248	1.208647	-0.284034
C	-1.018143	2.903213	-0.284017
N	-2.037486	0.067749	-0.239940
C	-4.223465	0.825003	-0.347207
C	-0.542709	4.268965	-0.347022
N	0.067751	2.037487	-0.239840
C	-2.903212	-1.018137	-0.284261
C	-4.268971	-0.542700	-0.347098
H	-5.050771	1.518394	-0.391110
C	0.824995	4.223476	-0.346922
H	-1.179544	5.140527	-0.391059
C	1.208645	2.829252	-0.283947
C	-2.516374	-2.354594	-0.290885
H	-5.140537	-1.179532	-0.391076
H	1.518382	5.050787	-0.390772
C	2.516377	2.354610	-0.290433
C	-1.208639	-2.829227	-0.284430
H	-3.308322	-3.095521	-0.326957
C	2.903214	1.018149	-0.284015
H	3.308329	3.095537	-0.326415
N	-0.067748	-2.037466	-0.240126
C	-0.824989	-4.223440	-0.347651
N	2.037488	-0.067750	-0.239920
C	4.268956	0.542723	-0.347309
C	1.018144	-2.903187	-0.284482
C	0.542713	-4.268930	-0.347714
H	-1.518377	-5.050743	-0.391645
C	2.829253	-1.208635	-0.284216
C	4.223489	-0.824981	-0.346886
H	5.140510	1.179564	-0.391414
C	2.354607	-2.516362	-0.290899
H	1.179551	-5.140483	-0.391868
H	5.050809	-1.518365	-0.390627
H	3.095529	-3.308316	-0.326959
Fe	-0.000001	-0.000001	0.231961
Cl	-0.000016	-0.000097	2.494572

$TS_{25(S)}$

E= -1643.848778au

C	3.590406	3.425056	-0.029174
H	4.663952	3.578097	-0.027676
C	2.754176	4.547070	-0.034772
H	3.191299	5.540196	-0.037248
C	1.351136	4.395384	-0.037516
H	0.712123	5.272123	-0.042227
C	0.793666	3.131338	-0.033999
H	-0.279026	2.983029	-0.036205
C	1.622676	1.954630	-0.027508
N	1.023708	0.764129	-0.023105
C	3.075974	2.123898	-0.025761
C	3.917485	0.918577	-0.021032
C	3.303608	-0.338553	-0.018885
H	1.826490	-0.033951	-0.019940

C	5.334150	0.928234	-0.019101
H	5.876596	1.868165	-0.020351
C	3.981980	-1.544305	-0.015693
H	3.450341	-2.490648	-0.015141
C	5.387508	-1.505246	-0.014123
H	5.956463	-2.430202	-0.011857
C	6.050835	-0.269402	-0.015639
H	7.135782	-0.241234	-0.014269
H	-3.792888	3.448276	2.327200
C	-3.178361	2.561529	2.271565
C	-2.619842	1.851496	3.297177
C	-2.795674	1.906004	1.042113
C	-1.897852	0.747446	2.707763
H	-2.688495	2.040878	4.358471
N	-2.008730	0.796641	1.324514
C	-3.141380	2.346302	-0.225969
C	-1.224200	-0.223867	3.429933
C	-2.726950	1.750975	-1.407031
H	-3.767357	3.228806	-0.299547
C	-0.577950	-1.315923	2.874379
H	-1.224054	-0.136522	4.510802
N	-1.933236	0.615338	-1.503459
C	-3.037409	2.246127	-2.728526
N	-0.480250	-1.595268	1.517571
C	0.071337	-2.356832	3.637661
C	-1.746987	0.392025	-2.861233
C	-2.428321	1.412690	-3.624079
H	-3.641767	3.118759	-2.929208
C	0.208138	-2.797970	1.422992
C	0.549495	-3.273338	2.743917
H	0.137389	-2.374587	4.715704
C	-1.042235	-0.663187	-3.417051
H	-2.437230	1.466753	-4.702915
C	0.544853	-3.443012	0.243406
H	1.086703	-4.188616	2.945555
C	-0.432934	-1.675351	-2.693807
H	-0.984697	-0.714202	-4.498729
C	0.269601	-2.957867	-1.025536
H	1.072448	-4.387652	0.318768
N	-0.406239	-1.778071	-1.309211
C	0.247970	-2.805402	-3.282747
C	0.674233	-3.599395	-2.255344
H	0.368700	-2.961574	-4.344779
H	1.214492	-4.533266	-2.310370
Fe	-1.368872	-0.591999	0.009550
Cl	-3.348715	-1.852636	0.041366

5(S)

E= -1643.8499014au

C	3.413074	3.480543	-0.095863
H	4.477085	3.685018	-0.113573
C	2.533313	4.567542	-0.105976
H	2.931189	5.576796	-0.126976
C	1.138596	4.357991	-0.091208
H	0.461235	5.205326	-0.099376
C	0.641957	3.070417	-0.069060
H	-0.422350	2.872610	-0.060538
C	1.515621	1.925417	-0.060040
N	0.933426	0.725281	-0.044012
C	2.961384	2.153864	-0.070000
C	3.896137	1.013259	-0.053386
C	3.449092	-0.307828	-0.086770
H	1.650269	-0.035929	-0.045791
C	5.309888	1.156803	-0.000753
H	5.754923	2.145024	0.037867
C	4.233913	-1.441963	-0.080380
H	3.798720	-2.435659	-0.111456
C	5.627108	-1.257876	-0.032208
H	6.290327	-2.117455	-0.024833
C	6.149803	0.042980	0.008485
H	7.224305	0.189337	0.049478
H	-3.974232	3.361472	2.229230
C	-3.317364	2.504338	2.197763
C	-2.727989	1.849342	3.242678
C	-2.900566	1.835314	0.986349
C	-1.951874	0.765707	2.683810
H	-2.809030	2.063127	4.298478
N	-2.062145	0.773793	1.300218

C	-3.263368	2.223499	-0.294418
C	-1.235185	-0.153910	3.432652
C	-2.820868	1.614691	-1.458822
H	-3.929692	3.073488	-0.392904
C	-0.537857	-1.230944	2.909053
H	-1.243284	-0.038001	4.510851
N	-1.975617	0.515453	-1.524132
C	-3.154645	2.055683	-2.794246
N	-0.421070	-1.541867	1.561220
C	0.152702	-2.222516	3.701793
C	-1.779911	0.259410	-2.874198
C	-2.508473	1.224799	-3.665932
H	-3.799169	2.892820	-3.019768
C	0.318232	-2.715922	1.499638
C	0.674341	-3.140550	2.834071
H	0.214038	-2.209725	4.780199
C	-1.029116	-0.780171	-3.399702
H	-2.521430	1.245836	-4.745959
C	0.685369	-3.377523	0.338098
H	1.249152	-4.026268	3.062142
C	-0.374557	-1.743826	-2.648893
H	-0.971898	-0.861527	-4.479661
C	0.387979	-2.943749	-0.944778
H	1.254352	-4.295167	0.440410
N	-0.337381	-1.802836	-1.262579
C	0.351256	-2.862430	-3.206051
C	0.814953	-3.605332	-2.156494
H	0.473655	-3.047318	-4.263351
H	1.392667	-4.517731	-2.185781
Fe	-1.341254	-0.610293	0.023172
Cl	-3.265082	-1.967622	0.092503

amine

E= -517.373718au

C	-1.137542	-0.860007	-0.000005
N	0.002126	-1.659752	0.000086
C	-0.726848	0.504826	0.000010
C	0.726763	0.504820	0.000011
C	1.135904	-0.859845	-0.000005
H	0.001689	-2.666090	0.000122
C	-2.488377	-1.223180	-0.000029
H	-2.793066	-2.264952	-0.000010
C	-1.699934	1.513802	-0.000001
H	-1.409113	2.559822	0.000002
C	-3.437608	-0.198037	-0.000029
C	-3.050308	1.157068	-0.000004
H	-3.811959	1.929880	0.000005
H	-4.492951	-0.451786	-0.000019
C	1.700266	1.514028	0.000001
H	1.409465	2.560098	0.000005
C	3.050253	1.157766	-0.000004
H	3.812062	1.930304	0.000005
C	2.488147	-1.224155	-0.000028
H	2.794599	-2.265916	-0.000010
C	3.436348	-0.197489	-0.000032
H	4.492007	-0.450687	-0.000023

N_2

E= -109.521579au

N	0.000000	0.000000	0.551961
N	0.000000	0.000000	-0.551961

2'(Q)

E= -1718.0578836au

N	0.076653	0.944245	-0.190336
C	0.172073	2.249554	-0.321770
C	1.467911	2.927858	-0.386415
C	2.754528	2.258235	-0.310967
C	3.013463	0.934325	-0.194077
H	2.232928	0.183606	-0.144765
C	-1.030422	3.045702	-0.411653
C	1.463367	4.326498	-0.526581
H	2.420058	4.837914	-0.571807
C	0.284636	5.070117	-0.608723
H	0.332215	6.148129	-0.716968
C	-0.964821	4.418548	-0.551494
H	-1.881220	4.995378	-0.617038
H	-1.978678	2.528371	-0.367269

C	2.305938	-3.106248	-1.403424
C	1.702322	-2.797975	-2.588830
C	1.530242	-2.476322	-0.354986
H	3.204676	-3.680211	-1.235353
C	0.545347	-1.984973	-2.276290
H	1.997523	-3.086981	-3.586975
N	0.457163	-1.796880	-0.910484
C	1.863257	-2.492246	0.990237
C	-0.357273	-1.492369	-3.209322
Fe	-0.985299	-0.813898	0.101235
C	1.180416	-1.815330	1.991805
H	2.754249	-3.039019	1.275218
C	-1.516384	-0.803099	-2.897220
H	-0.170274	-1.711630	-4.254983
Cl	-2.086284	-2.721811	0.464629
N	0.043987	-1.039700	1.819486
N	-2.386070	0.235997	1.100753
N	-1.931486	-0.446215	-1.614530
C	1.577617	-1.793942	3.381992
C	-2.527827	-0.427673	-3.857286
C	-0.283863	-0.546979	3.070316
C	-2.395942	0.547744	2.456614
C	-3.600858	0.674717	0.596903
C	-3.196648	0.111225	-1.761425
C	0.680049	-1.004013	4.045703
H	2.432571	-2.319509	3.781699
C	-3.565397	0.123397	-3.158765
H	-2.450413	-0.591591	-4.922301
C	-1.404601	0.218875	3.364833
C	-3.635004	1.212925	2.796069
C	-4.382269	1.280344	1.654686
C	-3.984425	0.610295	-0.735128
H	0.651743	-0.759616	5.097620
H	-4.501545	0.504433	-3.540652
H	-1.542971	0.529633	4.394800
H	-3.891700	1.560089	3.786421
H	-5.369860	1.698797	1.524303
H	-4.961324	1.001901	-0.997425
H	3.613133	2.923770	-0.355517
C	4.379518	0.401359	-0.117424
O	4.660992	-0.801278	0.013281
O	5.361918	1.372814	-0.200562
C	6.749706	0.903118	-0.125502
H	7.353867	1.805349	-0.200851
H	6.924713	0.389662	0.822570
H	6.961943	0.217262	-0.948765

$TS_{23'(Q)}$

E= -1718.0148951au

N	-0.145648	0.882733	-0.885074
C	-1.104036	1.716605	-1.387658
C	-0.651969	3.037186	-1.767121
C	0.774172	3.139304	-1.539144
C	1.417597	1.885556	-1.593655
C	-2.476350	1.403359	-1.540712
C	-1.551530	4.004366	-2.197979
H	-1.204183	5.003251	-2.441275
C	-2.911735	3.669435	-2.337344
H	-3.616607	4.414299	-2.690964
C	-3.355541	2.376814	-2.025604
H	-4.404138	2.125727	-2.146007
H	-2.837417	0.419519	-1.289288
H	1.305810	1.261897	-2.477553
H	4.074702	-0.625643	1.863277
C	3.055263	-0.610818	1.492956
C	2.150020	0.223293	2.133605
C	2.756493	-1.388140	0.383675
N	0.802005	0.322461	1.827928
C	2.477460	1.138905	3.203762
C	3.712172	-2.172382	-0.368457
N	1.510645	-1.466597	-0.219761
C	0.272783	1.260208	2.699635
Fe	-0.221197	-0.792912	0.522466
C	1.326570	1.794533	3.537576
H	3.464808	1.263778	3.623249
C	3.047176	-2.694610	-1.441815
H	4.752329	-2.294077	-0.102180
C	1.665264	-2.273782	-1.333353

C	−1.075759	1.553067	2.849415
Cl	−0.301759	−2.524136	1.972399
N	−1.960773	−0.103823	1.252064
N	−1.252246	−1.832669	−0.846925
H	1.182961	2.551302	4.295076
H	3.433589	−3.332521	−2.223662
C	0.640874	−2.715976	−2.160352
C	−2.111468	0.871912	2.223214
H	−1.344529	2.300389	3.588461
C	−3.227741	−0.616784	1.013320
C	−2.614471	−2.102050	−0.844894
C	−0.713878	−2.550425	−1.904287
H	0.915905	−3.332490	−3.009572
C	−3.510730	0.998763	2.573457
C	−4.194852	0.066272	1.844466
C	−3.533196	−1.568971	0.049959
C	−2.938414	−2.980250	−1.947346
C	−1.772126	−3.239181	−2.612452
H	−3.899495	1.693643	3.303785
H	−5.254509	−0.144623	1.853454
H	−4.568021	−1.880465	−0.043378
H	−3.930944	−3.343622	−2.171514
H	−1.622511	−3.864077	−3.481085
C	2.789850	1.830901	−1.012877
O	3.202883	2.522856	−0.073665
O	3.592840	0.979295	−1.729302
C	5.010662	0.931456	−1.346612
H	5.103367	0.703044	−0.284362
H	5.436543	0.140742	−1.959503
H	5.482593	1.894510	−1.556508
H	1.251740	4.008083	−1.099491

$TS_{25'(Q)}$

E= -1718.0235387au

C	−0.113260	4.508122	−1.490590
H	0.549714	5.343949	−1.691636
C	−1.496002	4.670045	−1.608673
H	−1.906128	5.631177	−1.899263
C	−2.357729	3.581703	−1.352510
H	−3.430425	3.709955	−1.450421
C	−1.852093	2.350381	−0.976929
H	−2.510812	1.519746	−0.784454
C	−0.435692	2.143580	−0.839864
N	0.075386	0.964753	−0.483956
C	0.444778	3.279698	−1.117449
C	1.872529	3.098541	−1.003810
C	2.403111	1.905220	−0.676209
H	1.283160	1.059006	−0.491691
C	3.837210	1.645814	−0.574664
H	−4.902432	1.033911	2.601255
C	−3.843871	0.859415	2.473029
C	−2.818464	1.242474	3.291326
C	−3.257254	0.158115	1.351065
C	−1.593120	0.749348	2.700562
H	−2.874366	1.782248	4.225503
N	−1.878909	0.110231	1.499725
C	−3.961498	−0.315640	0.251238
C	−0.347934	0.798372	3.308654
C	−3.378252	−0.838248	−0.896161
H	−5.041589	−0.216490	0.265451
C	0.772406	0.106097	2.864535
H	−0.270771	1.326542	4.252965
N	−2.016363	−1.028601	−1.084028
C	−4.087998	−1.171177	−2.112919
N	0.840921	−0.623735	1.691619
C	1.995442	−0.067156	3.619089
C	−1.862204	−1.492232	−2.384928
C	−3.153516	−1.551459	−3.035129
H	−5.160043	−1.110833	−2.233471
C	2.060019	−1.281661	1.707151
C	2.778233	−0.940910	2.916677
H	2.201590	0.399649	4.571274
C	−0.677339	−1.955120	−2.936967
H	−3.312418	−1.874181	−4.053854
C	2.550976	−2.085921	0.688676
H	3.755448	−1.320628	3.177810
C	0.501600	−2.143344	−2.225000
H	−0.702506	−2.296193	−3.966405

C	1.936516	-2.280893	-0.540145
H	3.522463	-2.543781	0.839435
N	0.701243	-1.775579	-0.907792
C	1.655697	-2.871074	-2.709390
C	2.528687	-2.976910	-1.662848
H	1.757061	-3.267456	-3.709232
H	3.490438	-3.468873	-1.642304
Fe	-0.600843	-0.850770	0.308235
Cl	-1.175828	-2.826992	1.214491
H	2.520616	3.952091	-1.205870
O	4.709904	2.532591	-0.541487
O	4.144638	0.311145	-0.535398
C	5.572509	-0.026470	-0.453549
H	5.597669	-1.113801	-0.434109
H	6.102405	0.364385	-1.324824
H	6.008723	0.396844	0.453871

5'(Q)

E=-1718.0321942au

C	0.606502	4.604776	-0.008962
H	1.398914	5.348191	-0.009602
C	-0.724623	5.016204	-0.011233
H	-0.965412	6.074012	-0.014018
C	-1.755568	4.053250	-0.009990
H	-2.792585	4.370860	-0.011509
C	-1.454323	2.704031	-0.006614
H	-2.238633	1.964735	-0.005141
C	-0.097048	2.245516	-0.004562
N	0.164656	0.925110	-0.001054
C	0.964733	3.246891	-0.005701
C	2.377976	2.921232	-0.003122
C	2.976068	1.722297	-0.000761
H	1.166090	0.700706	-0.000449
H	-5.119459	0.541284	2.636778
C	-4.079368	0.278979	2.506894
C	-3.121757	0.113305	3.467111
C	-3.447729	0.036196	1.227120
C	-1.897628	-0.258101	2.789903
H	-3.225055	0.204828	4.538653
N	-2.110322	-0.276592	1.418083
C	-4.076955	0.160491	-0.004494
C	-0.728203	-0.634698	3.432471
C	-3.445092	0.029905	-1.234093
H	-5.132394	0.410484	-0.006251
C	0.379844	-1.183431	2.800669
H	-0.709167	-0.572966	4.515255
N	-2.107276	-0.283755	-1.420668
C	-4.074132	0.265794	-2.516427
N	0.521717	-1.345147	1.433916
C	1.525671	-1.748969	3.480630
C	-1.891810	-0.272632	-2.792112
C	-3.114575	0.095034	-3.473787
H	-5.113982	0.527277	-2.649844
C	1.717584	-2.018498	1.239370
C	2.342206	-2.275840	2.519612
H	1.662579	-1.753339	4.552277
C	-0.720989	-0.652355	-3.430221
H	-3.215673	0.180746	-4.546009
C	2.265457	-2.351388	0.008682
H	3.283797	-2.789402	2.649339
C	0.385783	-1.197591	-2.793251
H	-0.699670	-0.596297	-4.513263
C	1.720231	-2.024604	-1.224850
H	3.217030	-2.870505	0.010982
N	0.524597	-1.352568	-1.425364
C	1.533244	-1.766203	-3.467809
C	2.347724	-2.288107	-2.502362
H	1.672479	-1.775939	-4.539111
H	3.289830	-2.801879	-2.627381
Fe	-0.806453	-0.824920	0.001416
Cl	-1.642952	-2.915315	0.007271
H	3.051719	3.785210	-0.003791
C	4.392803	1.401777	-0.000014
O	4.640316	0.055646	-0.007980
C	6.055666	-0.348096	-0.006169
H	6.031289	-1.435522	0.005210
H	6.553848	0.026577	-0.902861
H	6.557939	0.046026	0.879705

O	5.297274	2.257212	0.006812

2'(S)

E= -1718.0661029au

N	-0.444713	1.285226	-0.656757
C	-0.679252	2.573707	-0.792291
C	-2.029590	3.133479	-0.811423
C	-3.236380	2.340797	-0.669389
C	-3.362456	1.005350	-0.478031
H	-2.519981	0.326727	-0.399256
C	0.446233	3.468772	-0.936038
C	-2.157405	4.523109	-0.979907
H	-3.156468	4.948094	-0.999332
C	-1.050673	5.363941	-1.119597
H	-1.196694	6.431127	-1.246140
C	0.255056	4.827941	-1.094897
H	1.111704	5.485041	-1.201827
H	1.438193	3.033131	-0.914013
C	-4.709886	0.430668	-0.370959
C	-2.357530	-2.254942	2.219869
C	-1.864227	-1.455439	3.211661
C	-1.452864	-2.151091	1.099687
H	-3.252210	-2.859059	2.227088
C	-0.655097	-0.848194	2.706302
H	-2.271787	-1.278726	4.196260
N	-0.414103	-1.280676	1.408378
C	-1.611577	-2.822375	-0.100243
C	0.132478	0.039599	3.419282
Fe	1.223394	-0.905906	0.291406
C	-0.753371	-2.715633	-1.181165
H	-2.476321	-3.466617	-0.205420
C	1.275403	0.646174	2.927972
H	-0.170662	0.280935	4.432004
Cl	2.523455	-2.664875	1.102310
N	0.387773	-1.925093	-1.233514
N	2.596340	-0.163986	-0.991402
N	1.809056	0.459661	1.656987
C	-0.931637	-3.407273	-2.436420
C	2.087417	1.580402	3.670855
C	0.920936	-2.111995	-2.502283
C	2.831315	-0.589743	-2.294411
C	3.621147	0.728167	-0.693941
C	2.944103	1.261221	1.602049
C	0.101301	-3.036617	-3.250166
H	-1.746284	-4.082917	-2.652015
C	3.115421	1.959484	2.854189
H	1.885696	1.894424	4.684532
C	2.058679	-1.497729	-2.997463
C	4.012203	0.055064	-2.817728
C	4.498630	0.867558	-1.832162
C	3.788086	1.389760	0.511592
H	0.301342	-3.348715	-4.264737
H	3.922824	2.644851	3.067085
H	2.363000	-1.741178	-4.009323
H	4.407529	-0.105192	-3.810155
H	5.371886	1.503048	-1.857491
H	4.641881	2.051047	0.610147
H	-4.166915	2.904466	-0.724540
O	-5.786544	1.048270	-0.432049
O	-4.663825	-0.939805	-0.192785
C	-5.961064	-1.619103	-0.089035
H	-6.544552	-1.460719	-0.998742
H	-5.716863	-2.671727	0.041395
H	-6.522224	-1.235632	0.766053

$TS_{23'(S)}$

E= -1718.0257001au

N	1.971419	0.438940	-1.374445
C	2.977578	-0.435245	-1.128658
C	4.240939	0.109031	-0.678484
C	4.141895	1.565922	-0.648169
C	2.829720	2.020963	-0.450114
C	2.861449	-1.834070	-1.340195
C	5.331872	-0.725922	-0.477368
H	6.288721	-0.314664	-0.171474
C	5.186488	-2.116431	-0.665692
H	6.033607	-2.771687	-0.491566
C	3.961446	-2.657579	-1.085744

H	3.868960	-3.729185	-1.229299
H	1.920900	-2.242068	-1.690695
C	2.451687	3.351312	-0.984582
H	2.239229	1.686469	0.398440
H	-0.857576	3.160216	3.029594
C	-0.940311	2.300322	2.374663
C	-1.738272	2.420331	1.251232
C	-0.231249	1.161974	2.713966
N	-1.953132	1.429279	0.300727
C	-2.460525	3.616879	0.889612
C	0.613048	1.043336	3.878462
N	-0.228388	-0.032901	1.999602
C	-2.792761	1.995857	-0.651528
Fe	-1.413665	-0.507791	0.436436
C	-3.109047	3.355834	-0.285131
H	-2.465885	4.526905	1.471777
C	1.122089	-0.224775	3.879779
H	0.782163	1.834632	4.593972
C	0.594585	-0.896537	2.716465
C	-3.258790	1.365310	-1.791502
Cl	-3.257025	-1.235750	1.646039
N	-2.156190	-0.809530	-1.414367
N	-0.471625	-2.287331	0.310967
H	-3.749336	4.010172	-0.858542
H	1.790756	-0.678203	4.596717
C	0.868901	-2.210492	2.381351
C	-2.953070	0.063958	-2.147026
H	-3.904809	1.930901	-2.453481
C	-2.143284	-1.999160	-2.135187
C	-0.700915	-3.285860	-0.630931
C	0.370836	-2.854015	1.262278
H	1.521214	-2.773562	3.039275
C	-3.431464	-0.587556	-3.343043
C	-2.932858	-1.859152	-3.335544
C	-1.477541	-3.155434	-1.769190
C	0.008478	-4.486888	-0.259904
C	0.668931	-4.220314	0.906893
H	-4.065460	-0.119915	-4.081937
H	-3.077129	-2.640665	-4.067033
H	-1.565923	-4.016777	-2.421783
H	-0.008881	-5.406856	-0.825851
H	1.301285	-4.878033	1.485057
H	4.889343	2.206209	-1.107022
O	3.122342	4.031972	-1.774803
O	1.226516	3.753454	-0.510019
C	0.699507	5.018616	-1.039032
H	0.726623	5.008698	-2.130616
H	-0.322035	5.067452	-0.668809
H	1.297346	5.856367	-0.671610

5'(S)

E=-1718.0328736au

C	-1.531949	4.763346	-0.146293
H	-2.416388	5.393446	-0.160458
C	-0.266344	5.352438	-0.158167
H	-0.174601	6.433054	-0.181934
C	0.893926	4.544197	-0.138607
H	1.874112	5.008868	-0.147330
C	0.781454	3.168818	-0.108700
H	1.653486	2.528012	-0.093307
C	-0.505922	2.518475	-0.097109
N	-0.520713	1.190784	-0.070604
C	-1.697772	3.368059	-0.115629
C	-3.037046	2.820844	-0.102038
C	-3.392662	1.527727	-0.072184
H	-1.484293	0.817779	-0.064109
C	-4.713835	0.929372	-0.054364
H	5.178325	1.485241	-2.177309
C	4.229286	0.969891	-2.148251
C	3.466512	0.539181	-3.197530
C	3.530865	0.607020	-0.936546
C	2.297114	-0.101298	-2.640627
H	3.668897	0.630691	-4.254753
N	2.345617	-0.044979	-1.253443
C	3.971535	0.899232	0.345179
C	1.299693	-0.702174	-3.391142
C	3.278161	0.593256	1.506099
H	4.920723	1.413807	0.446461

C	0.206431	-1.371487	-2.863948
H	1.395094	-0.669094	-4.470923
N	2.059068	-0.069111	1.567361
C	3.714158	0.941639	2.838954
N	-0.073597	-1.524807	-1.513585
C	-0.801874	-2.042208	-3.652526
C	1.731527	-0.147279	2.914922
C	2.758893	0.490533	3.706002
H	4.633412	1.461584	3.066307
C	-1.232481	-2.287189	-1.444615
C	-1.684835	-2.611074	-2.777865
H	-0.814862	-2.072111	-4.732315
C	0.610133	-0.768045	3.440501
H	2.742623	0.566557	4.783456
C	-1.879476	-2.667040	-0.279799
H	-2.565418	-3.195748	-3.000518
C	-0.350608	-1.431857	2.694156
H	0.488273	-0.755360	4.517992
C	-1.475629	-2.317523	0.998593
H	-2.779278	-3.263359	-0.377067
N	-0.358586	-1.553588	1.311821
C	-1.488576	-2.125170	3.253190
C	-2.178154	-2.674897	2.208946
H	-1.713316	-2.181383	4.308312
H	-3.080946	-3.267032	2.240432
Fe	1.084685	-0.948403	0.035960
Cl	2.299973	-2.961615	0.145737
H	-3.851052	3.553606	-0.117561
O	-5.778070	1.575423	-0.060041
O	-4.676620	-0.442020	-0.029791
C	-5.978174	-1.127255	-0.007737
H	-5.731762	-2.186604	0.014687
H	-6.543170	-0.834288	0.879758
H	-6.552322	-0.874235	-0.901685

$TS_{25'(S)}$

E= -1718.0288414au

C	1.805271	4.925312	-0.251021
H	2.695149	5.547607	-0.253434
C	0.539912	5.520030	-0.283873
H	0.453350	6.601063	-0.311264
C	-0.627333	4.721062	-0.281161
H	-1.602072	5.196704	-0.306306
C	-0.535788	3.342376	-0.246219
H	-1.418709	2.715971	-0.241325
C	0.749722	2.690922	-0.211739
N	0.809045	1.366956	-0.178512
C	1.948266	3.533019	-0.214919
C	3.237820	2.881417	-0.181685
C	3.334949	1.537843	-0.149369
H	1.921896	1.057620	-0.156817
C	4.567530	0.762564	-0.118361
H	-4.801518	2.088197	2.229613
C	-3.906268	1.484094	2.204479
C	-3.104583	1.112685	3.247384
C	-3.337218	0.914034	1.006168
C	-2.041530	0.302852	2.700722
H	-3.214891	1.350939	4.295226
N	-2.190347	0.193309	1.322757
C	-3.848376	1.093500	-0.269372
C	-1.043273	-0.291425	3.453581
C	-3.268836	0.595740	-1.424727
H	-4.756132	1.677914	-0.371696
C	-0.051136	-1.109511	2.939904
H	-1.051096	-0.121088	4.524456
N	-2.115870	-0.179139	-1.481659
C	-3.766446	0.836974	-2.758684
N	0.108424	-1.445413	1.601302
C	0.961104	-1.764057	3.735700
C	-1.893019	-0.428711	-2.831109
C	-2.915009	0.211263	-3.625320
H	-4.651500	1.412732	-2.987089
C	1.197152	-2.306954	1.552872
C	1.726010	-2.507087	2.881503
H	1.056799	-1.663662	4.806972
C	-0.866172	-1.198858	-3.349453
H	-2.966109	0.171393	-4.703572
C	1.720979	-2.877467	0.406027

H	2.574660	-3.133443	3.114375
C	0.086994	-1.854318	-2.588811
H	-0.816545	-1.313003	-4.426608
C	1.254208	-2.638439	-0.874804
H	2.572900	-3.538628	0.516705
N	0.176131	-1.826041	-1.202923
C	1.129819	-2.692933	-3.132309
C	1.844406	-3.181609	-2.075426
H	1.279086	-2.877967	-4.186003
H	2.696923	-3.844689	-2.092517
Fe	-1.134863	-0.994723	0.080669
Cl	-2.500253	-2.877369	0.299960
O	5.715798	1.242608	-0.102672
O	4.337149	-0.593288	-0.109488
H	4.135283	3.502322	-0.184704
C	5.528559	-1.451832	-0.085376
H	6.149236	-1.261613	-0.963771
H	6.114247	-1.260174	0.816553
H	5.138236	-2.467331	-0.092612

1(Q)-[Fe^{III}(F_{20}TPP)Cl]

E=-4661.4771873au

N	0.000030	-0.016107	2.168037
C	0.555267	-0.937671	3.118387
C	-0.179064	-1.545708	4.165994
C	-1.643707	-1.339294	4.360066
C	-2.554927	-1.621476	3.324313
H	-2.182766	-1.989872	2.372714
N	-0.841565	0.816435	2.536441
N	-1.608773	1.643374	2.689969
C	1.911729	-1.240022	2.929689
H	2.444413	-0.761806	2.117849
C	0.516353	-2.408141	5.034596
H	-0.037163	-2.881319	5.839354
C	2.569541	-2.118561	3.791157
C	1.871991	-2.695645	4.857995
H	3.618812	-2.338003	3.628881
H	2.373876	-3.375211	5.538798
C	-2.146370	-0.907045	5.601828
H	-1.452373	-0.681619	6.405805
C	-3.928892	-1.459036	3.523625
H	-4.617839	-1.679688	2.713486
C	-4.416229	-1.021287	4.760815
C	-3.520919	-0.749398	5.801028
H	-5.483260	-0.894120	4.913354
H	-3.890552	-0.408459	6.762835
C	-2.874677	1.832663	-0.820923
C	-1.722927	2.599315	-0.665154
C	-2.869337	0.439320	-0.847074
N	-0.423597	2.109832	-0.560774
C	-1.717876	4.037076	-0.538984
C	-4.062072	-0.373402	-0.887920
N	-1.743225	-0.373934	-0.794561
C	0.384558	3.227085	-0.373259
C	-0.427331	4.420586	-0.340381
H	-2.588867	4.669144	-0.588087
C	-3.664077	-1.676162	-0.858302
H	-5.070698	0.005088	-0.920028
C	-2.220485	-1.680136	-0.815169
C	1.773735	3.226627	-0.275274
H	-0.058333	5.421394	-0.188892
H	-4.287995	-2.555284	-0.870922
C	-1.443543	-2.835824	-0.819982
C	2.554435	2.078768	-0.393575
C	-0.051078	-2.831589	-0.821870
N	2.083001	0.783091	-0.568145
C	3.998595	2.081233	-0.395917
N	0.763041	-1.704920	-0.794426
C	0.760216	-4.025054	-0.878867
C	3.214770	-0.019055	-0.674728
C	4.404348	0.794020	-0.577279
H	4.619327	2.955702	-0.290204
C	2.067406	-2.182754	-0.842668
C	2.062444	-3.625953	-0.895532
H	0.380793	-5.033752	-0.907639
C	3.223365	-1.405155	-0.811570
H	5.415853	0.427397	-0.642912
H	2.940376	-4.250391	-0.931001
Fe	0.179806	0.218988	-0.909053

Cl	0.270760	0.386525	-3.212634
C	-4.189695	2.533783	-0.931051
C	-4.892159	2.575961	-2.141282
C	-4.782572	3.171597	0.164758
C	-6.120912	3.220306	-2.261582
C	-6.007948	3.825513	0.066013
C	-6.679939	3.848632	-1.152624
C	2.471684	4.529593	-0.056783
C	2.581380	5.489997	-1.068703
C	3.055219	4.844475	1.175678
C	3.233924	6.703973	-0.869548
C	3.716591	6.049446	1.396663
C	3.805148	6.983604	0.368530
C	4.543849	-2.102889	-0.874965
C	5.031726	-2.645001	-2.069615
C	5.349602	-2.252045	0.258989
C	6.258426	-3.301848	-2.136173
C	6.579771	-2.901795	0.216936
C	7.035098	-3.429247	-0.988183
C	-2.143130	-4.157938	-0.841527
C	-2.657484	-4.699631	-2.024336
C	-2.308918	-4.912085	0.324467
C	-3.305615	-5.932493	-2.049974
C	-2.951431	-6.147249	0.323543
C	-3.451216	-6.658339	-0.871170
F	-4.366320	1.963776	-3.255954
F	-6.781326	3.241799	-3.465383
F	-7.888688	4.487717	-1.259777
F	-6.558878	4.441403	1.163588
F	-4.145943	3.164749	1.386014
F	2.981957	3.941434	2.213839
F	4.276406	6.322761	2.620835
F	4.452785	8.174673	0.574817
F	3.321539	7.622173	-1.886922
F	2.029560	5.242769	-2.305665
F	-1.827454	-4.424874	1.522115
F	-3.097045	-6.860323	1.488314
F	-4.086705	-7.873446	-0.886002
F	-3.798450	-6.436400	-3.228222
F	-2.527353	-4.005098	-3.204760
F	4.926199	-1.739791	1.471102
F	7.341141	-3.028956	1.353200
F	8.244557	-4.072723	-1.043297
F	6.707093	-3.820812	-3.325199
F	4.287625	-2.534839	-3.221282

$TS_{12(Q)}$-[$Fe^{III}(F_{20}TPP)Cl$]

E= -4661.42352619au

N	-0.069609	-0.523080	2.156048
C	0.779702	-0.972177	3.131772
C	0.377183	-1.490448	4.414623
C	-1.040241	-1.491891	4.857536
C	-2.054381	-2.054125	4.054226
H	-1.796093	-2.470111	3.086053
N	-1.174527	0.641772	2.768022
N	-2.133139	1.121351	2.448046
C	2.160285	-1.007832	2.781751
H	2.448736	-0.581922	1.829371
C	1.368705	-1.985804	5.271660
H	1.073308	-2.372173	6.241850
C	3.108201	-1.577984	3.625379
C	2.714108	-2.049976	4.884493
H	4.146812	-1.623259	3.317971
H	3.448749	-2.469092	5.564564
C	-3.373650	-2.100126	4.510804
H	-4.142494	-2.545908	3.886777
C	-1.388787	-0.980741	6.124002
H	-0.618836	-0.534794	6.746116
C	-3.707975	-1.580876	5.768215
C	-2.710907	-1.021090	6.574446
H	-2.961882	-0.613385	7.548490
H	-4.735553	-1.613642	6.116275
H	4.374812	3.212530	-0.352168
C	3.803097	2.308927	-0.487899
C	2.363574	2.215610	-0.419427
C	4.274518	1.065569	-0.783884
N	1.963501	0.906286	-0.654186
C	1.520481	3.306827	-0.215406

C	3.133702	0.183893	-0.866946
H	5.301256	0.772805	-0.930389
Fe	0.090752	0.244061	-0.965148
C	0.133262	3.238042	-0.324473
C	3.214018	-1.194153	-1.061364
Cl	0.144161	0.455602	-3.270682
N	-1.787953	-0.452484	-0.840685
N	-0.609021	2.090579	-0.582833
N	0.781164	-1.639956	-0.892006
C	-0.741709	4.386172	-0.269391
C	2.104808	-2.039175	-1.027284
C	-2.195015	-1.780519	-0.801281
C	-2.952727	0.298971	-0.928949
C	-1.927160	2.515154	-0.716644
C	0.033969	-2.810039	-0.846458
C	-2.001635	3.946472	-0.539540
H	-0.430608	5.397615	-0.066037
C	2.180488	-3.481019	-1.066367
C	-3.637283	-1.852617	-0.842546
C	-1.355432	-2.891729	-0.776316
C	-4.101781	-0.576129	-0.942096
C	-3.031188	1.690720	-0.922572
C	0.909237	-3.954881	-0.943113
H	-2.901510	4.535855	-0.600106
H	3.087996	-4.055001	-1.159815
H	-4.216940	-2.760504	-0.806291
H	-5.128691	-0.252857	-0.993583
H	0.590700	-4.984547	-0.933421
C	4.561657	-1.810580	-1.247231
C	4.952687	-2.364931	-2.472416
C	5.493050	-1.877060	-0.204915
C	6.202554	-2.952579	-2.653520
C	6.748761	-2.455429	-0.362219
C	7.104338	-2.996869	-1.594227
C	2.148577	4.628716	0.088158
C	2.211591	5.658235	-0.857783
C	2.715088	4.889713	1.341223
C	2.801715	6.887639	-0.575365
C	3.314067	6.109270	1.644811
C	3.356467	7.112763	0.681234
C	-4.376846	2.318821	-1.087011
C	-5.033222	2.307622	-2.324106
C	-5.049128	2.932862	-0.024009
C	-6.290221	2.880398	-2.500355
C	-6.304259	3.515614	-0.178429
C	-6.927427	3.488032	-1.422514
C	-1.975654	-4.249878	-0.706882
C	-2.617950	-4.831193	-1.806061
C	-1.933895	-5.006608	0.468942
C	-3.193032	-6.098135	-1.741522
C	-2.497963	-6.276118	0.557122
C	-3.130789	-6.823720	-0.555266
F	1.675846	5.466088	-2.111833
F	2.844218	7.875259	-1.529008
F	3.942103	8.319217	0.969161
F	3.857772	6.328490	2.887247
F	2.686360	3.917425	2.317141
F	5.171956	-1.350531	1.032569
F	7.632379	-2.500512	0.689096
F	8.337890	-3.571893	-1.762507
F	6.551454	-3.484968	-3.870013
F	4.085448	-2.338901	-3.539873
F	-1.315878	-4.489082	1.589870
F	-2.436890	-6.986992	1.730986
F	-3.692225	-8.072934	-0.481990
F	-3.815705	-6.636740	-2.840681
F	-2.694641	-4.141007	-2.994410
F	-4.463895	2.974229	1.223445
F	-6.931884	4.110099	0.889944
F	-8.165102	4.056714	-1.585465
F	-6.902649	2.851930	-3.729172
F	-4.431087	1.713957	-3.409477