Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Unveiling the mechanism and regioselectivity of iron-dipyrrinato-catalyzed intramolecular C(sp^3)–H amination of alkyl azides

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Table of Contents

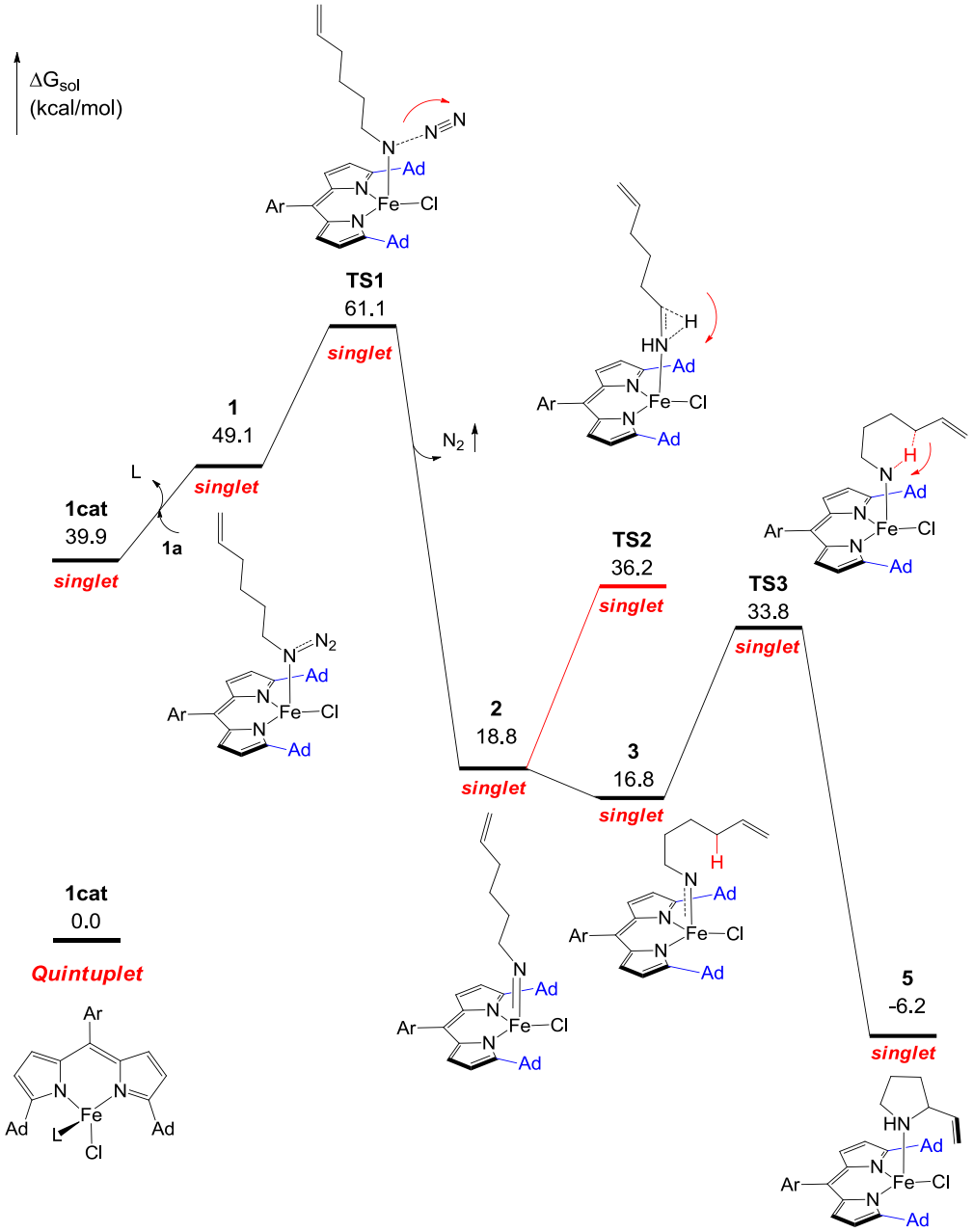

Fig. S1 Free energy profiles for iron-catalyzed direct amination of aliphatic C(sp^3)–H bond leading to pyrrolidine product. Energies are relative to **1cat** (quintuplet), and are mass balanced.

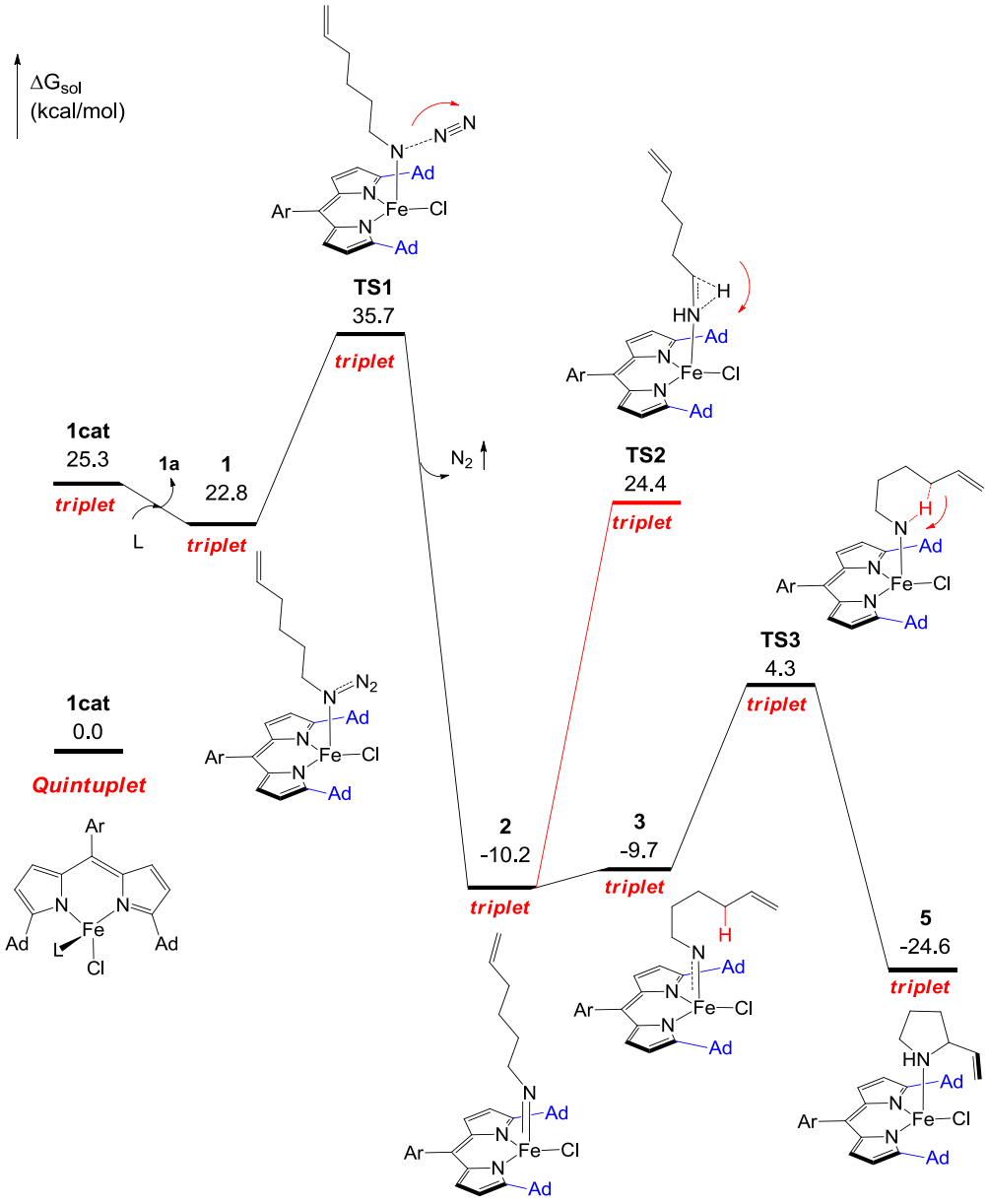

Fig. S2 Free energy profiles for iron-catalyzed direct amination of aliphatic C(sp^3)–H bond leading to pyrrolidine product. Energies are relative to **1cat** (quintuplet), and are mass balanced.

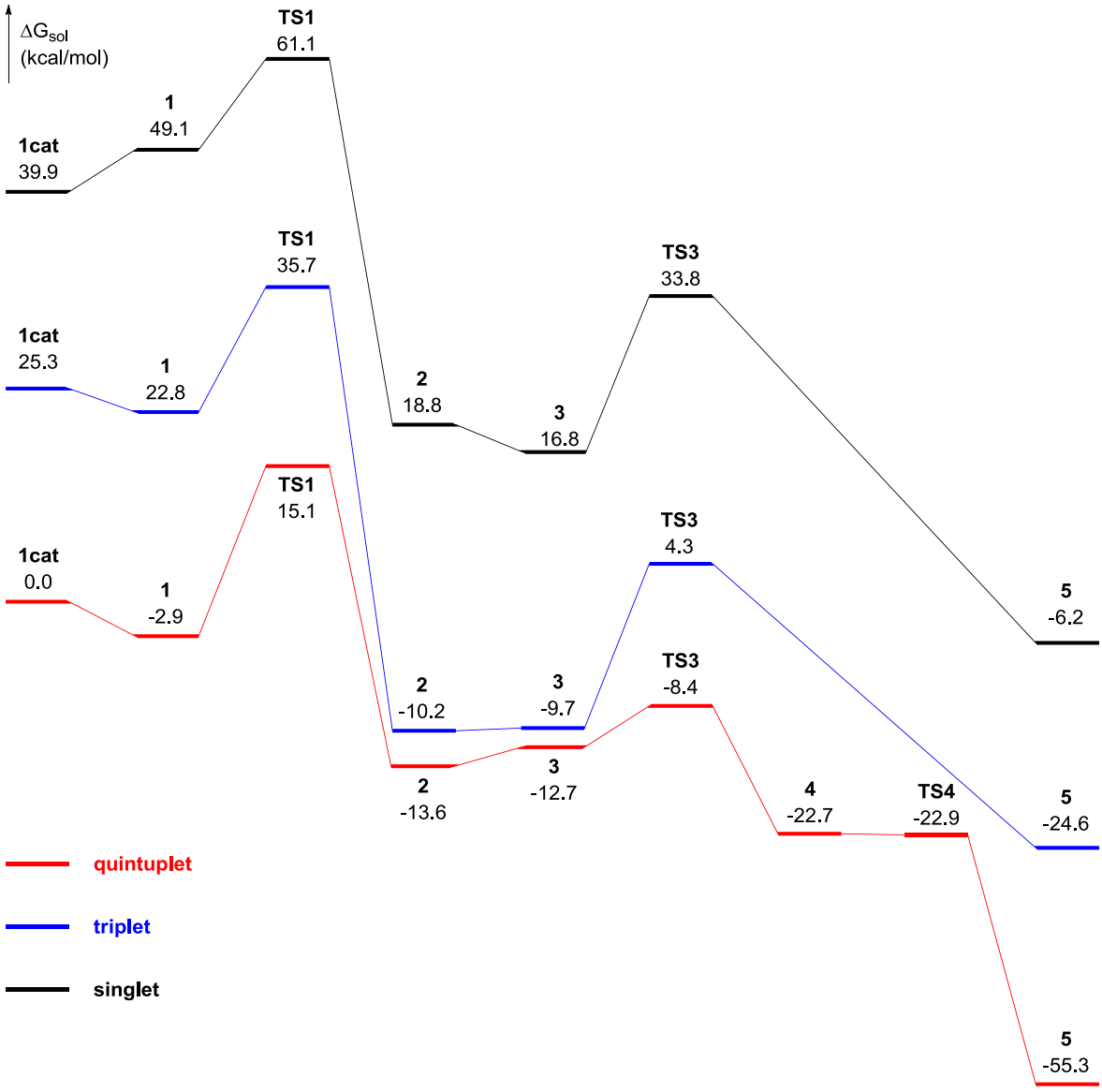

Fig. S3 Free energy profiles for iron-catalyzed direct amination of aliphatic C(sp^3)–H bond leading to pyrrolidine product. Energies are relative to **1cat** (quintuplet), and are mass balanced.

Cartesian Coordinates (Å), SCF Energies and Free Energies at 298.15 K and 1 atm for the Optimized Structures

1cat (quintuplet)

(U)B3LYP/BS1 SCF energy: -3203.88644 a.u.

(U)M06-L/BS2 SCF energy: -3203.768128 a.u.

(U)M06-L/BS2 Free energy: -3203.056873 a.u.

Fe	-0.020236	-0.793236	-0.052604
Cl	-0.168569	-2.801322	-1.145019
O	-0.101400	-1.222569	2.078290
N	1.590373	0.459016	-0.192391
N	-1.563108	0.595620	-0.202778
C	-2.916093	0.550791	-0.241087
C	-3.453438	1.873142	-0.220668
H	-4.500747	2.132576	-0.241050
C	-2.392618	2.744668	-0.175759
C	-1.202459	1.955198	-0.172149
C	2.939213	0.289537	-0.247223
C	-3.747378	-0.713873	-0.364069
C	-3.356559	-1.776839	0.697757
H	-2.299854	-2.036891	0.598522
C	-5.257621	-0.395761	-0.174636
H	-5.422320	0.054081	0.813408
H	-5.577877	0.340711	-0.921435
C	-3.571850	-1.328316	-1.786375
H	-3.870786	-0.583158	-2.535378
H	-2.518990	-1.563762	-1.963159
C	-4.427912	-2.604256	-1.933370
H	-4.273300	-3.019175	-2.937357
H	2.078106	-2.245092	0.538593
C	-0.157686	-0.132326	3.029362
H	-0.544580	0.712500	2.456393
C	1.194483	0.205672	3.642318
H	1.922598	0.451676	2.865246
C	0.151567	-2.545320	2.612526
H	1.126382	-2.548583	3.113242
H	0.219923	-3.180435	1.727444
H	2.338177	-1.766560	-1.989281
C	1.353620	1.842882	-0.157651
H	-2.434398	3.823826	-0.151524
C	0.098239	2.484218	-0.149676
C	3.587712	1.553338	-0.224920
C	3.645383	-1.046744	-0.388351
H	-3.494200	-1.351100	1.701279
C	-4.209499	-3.052836	0.536054
C	-6.116781	-1.667848	-0.324997
C	-5.916241	-2.257334	-1.735405
C	-3.996683	-3.640330	-0.874776
C	3.152986	-2.082614	0.656634
H	-0.896524	-0.375803	3.800322
H	1.082800	1.078825	4.293487
H	1.590909	-0.611115	4.253194
C	-0.945877	-3.049221	3.540696
C	3.409607	-1.628743	-1.816707
C	2.605009	2.519167	-0.169245
C	0.166640	3.989706	-0.144174
H	4.653380	1.721467	-0.254555
C	5.177645	-0.872922	-0.197334
H	-3.897411	-3.787668	1.290332
C	-5.697442	-2.706417	0.733494
H	-7.171840	-1.400183	-0.182283
H	-6.243275	-1.535742	-2.495974
H	-6.536068	-3.155189	-1.859777
H	-2.943722	-3.906282	-1.017467
H	-4.586913	-4.559608	-0.987370
H	3.318340	-1.687105	1.667899
C	3.884955	-3.430067	0.483476
H	-0.730798	-4.090319	3.803388
H	-1.920742	-3.016597	3.047356
H	-1.005797	-2.483302	4.474820
C	4.146428	-2.975481	-1.979816
H	3.770530	-0.906404	-2.560462

H	2.745531	3.590048	-0.148339
C	0.191038	4.732019	1.048613
C	0.213687	4.729706	-1.339901
H	5.564204	-0.161283	-0.936688
H	5.383435	-0.449823	0.794853
C	5.914454	-2.217320	-0.361014
H	-6.313051	-3.610743	0.640358
H	-5.865569	-2.306679	1.742828
C	3.621621	-3.980339	-0.933811
C	5.397775	-3.222444	0.686598
H	3.504815	-4.139620	1.230324
C	5.660423	-2.769688	-1.778272
H	3.955005	-3.362146	-2.988660
C	0.258767	6.124848	1.063814
C	0.281523	6.122930	-1.351381
H	6.989783	-2.051705	-0.215475
H	2.548813	-4.147945	-1.079892
H	4.124702	-4.948679	-1.057208
H	5.927999	-4.178724	0.587466
H	5.598970	-2.849110	1.700045
H	6.053003	-2.072263	-2.530195
H	6.194077	-3.719655	-1.914269
H	0.275351	6.650507	2.011467
C	0.303942	6.816663	-0.144039
H	0.316151	6.647926	-2.298964
H	0.356848	7.900857	-0.144197
Cl	0.134510	3.906333	2.600322
Cl	0.187702	3.900932	-2.884769

1 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3369.649906 a.u.

(U)M06-L/BS2 SCF energy: -3369.535007 a.u.

(U)M06-L/BS2 Free energy: -3368.80115 a.u.

Fe	-0.119670	-1.100597	-0.223233
Cl	-0.544333	-3.326021	-0.461845
N	1.548428	-0.087975	-0.780402
N	-1.577173	0.323214	-0.719691
C	-2.929625	0.392930	-0.699811
C	-3.360943	1.701138	-1.079635
H	-4.384310	2.036013	-1.148778
C	-2.236415	2.442685	-1.342403
C	-1.111935	1.587520	-1.127537
C	2.875289	-0.391220	-0.813975
C	-3.868607	-0.755922	-0.371157
C	-3.520942	-1.418919	0.990012
H	-2.498153	-1.802209	0.969011
C	-5.335560	-0.246972	-0.283533
H	-5.414439	0.531428	0.486820
H	-5.625865	0.211419	-1.236599
C	-3.816495	-1.841601	-1.489225
H	-4.085177	-1.379145	-2.448160
H	-2.798513	-2.227691	-1.587302
C	-4.786577	-2.997731	-1.165222
H	-4.716650	-3.748978	-1.961942
H	1.852515	-2.456257	0.764680
H	1.999960	-2.819356	-1.791060
C	1.423314	1.255320	-1.167392
H	-2.192774	3.474963	-1.657494
C	0.222839	1.979288	-1.315859
C	3.620768	0.751167	-1.204653
C	3.456945	-1.765644	-0.542348
H	-3.573617	-0.660455	1.783857
C	-4.489977	-2.578774	1.301108
C	-6.308588	-1.399792	0.036073
C	-6.228413	-2.460656	-1.079963
C	-4.398612	-3.638654	0.183480
C	2.942837	-2.366810	0.793763
C	3.087921	-2.740111	-1.703735
C	2.721429	1.774456	-1.425531
C	0.405877	3.401837	-1.777739
H	4.693300	0.802329	-1.313091
C	5.007443	-1.693465	-0.462520
H	-4.205388	-3.030445	2.260402
C	-5.929931	-2.038500	1.386239
H	-7.327975	-0.996083	0.090566

H	-6.528563	-2.020701	-2.040473
H	-6.927539	-3.281423	-0.871926
H	-3.381904	-4.042452	0.129468
H	-5.073081	-4.475774	0.407773
H	3.199861	-1.691130	1.620957
C	3.546016	-3.766273	1.035885
C	3.697052	-4.135549	-1.452157
H	3.461482	-2.325865	-2.649376
H	2.946862	2.782034	-1.743237
C	0.573179	4.463903	-0.873264
C	0.421947	3.738117	-3.143768
H	5.407261	-1.291661	-1.401438
H	5.306108	-1.002409	0.336710
C	5.616245	-3.087511	-0.211499
H	-6.626637	-2.851464	1.629138
H	-6.011557	-1.296096	2.191922
C	3.152502	-4.703267	-0.125125
C	5.080433	-3.656661	1.116533
H	3.150620	-4.162738	1.979660
C	5.232431	-4.027881	-1.371936
H	3.413814	-4.798466	-2.279402
C	0.744159	5.783823	-1.289194
C	0.591477	5.050359	-3.585557
H	6.708504	-2.991705	-0.158955
H	2.062539	-4.801009	-0.176537
H	3.563850	-5.706065	0.050473
H	5.520654	-4.643562	1.310272
H	5.373331	-3.006800	1.952372
H	5.637663	-3.643960	-2.317675
H	5.673886	-5.020704	-1.214519
H	0.867940	6.567092	-0.550431
C	0.752149	6.071178	-2.651928
H	0.596189	5.259117	-4.649053
H	0.884229	7.094987	-2.987506
Cl	0.570672	4.152516	0.857541
Cl	0.224484	2.486872	-4.356022
N	-0.188020	-0.826239	1.991076
C	-0.594589	0.417353	2.714227
C	0.570022	1.087948	3.445372
H	-1.410404	0.174178	3.406113
H	-0.996614	1.065114	1.934262
C	0.116138	2.333554	4.218667
H	1.027717	0.372696	4.142549
H	1.339491	1.357222	2.712627
C	1.281206	3.050332	4.928109
H	-0.373705	3.037616	3.534517
H	-0.641786	2.048393	4.961450
H	1.782030	2.330723	5.592980
H	2.026132	3.362908	4.186072
N	0.269663	-2.751746	3.314709
N	0.047587	-1.805736	2.726587
C	0.830670	4.241648	5.729026
C	1.207988	5.501120	5.508825
H	0.132379	4.032130	6.541114
H	0.843238	6.322366	6.118735
H	1.900738	5.756966	4.710164

TS1 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3369.611623 a.u.

(U)M06-L/BS2 SCF energy: -3369.504943 a.u.

(U)M06-L/BS2 Free energy: -3368.772401 a.u.

Fe	-0.316092	-0.815396	-0.195990
Cl	-0.807397	-2.924850	-0.827570
N	1.295786	0.104678	-1.054085
N	-1.724228	0.638247	-0.470882
C	-3.069716	0.740979	-0.273171
C	-3.471969	2.096066	-0.417539
H	-4.479397	2.469579	-0.320967
C	-2.347035	2.837002	-0.704724
C	-1.250011	1.933842	-0.746962
C	2.577152	-0.255545	-1.346851
C	-4.015563	-0.408616	0.024900
C	-3.543432	-1.238415	1.250288
H	-2.546389	-1.644030	1.069182
C	-5.436800	0.135833	0.345686

H	-5.388984	0.817537	1.204798
H	-5.813580	0.715185	-0.506147
C	-4.145283	-1.350225	-1.211938
H	-4.505347	-0.765905	-2.068952
H	-3.165339	-1.751865	-1.481193
C	-5.122354	-2.505785	-0.907493
H	-5.180400	-3.157713	-1.788228
H	1.797224	-2.455911	0.180369
H	1.369417	-2.499346	-2.417552
C	1.218917	1.501786	-1.199419
H	-2.293233	3.901013	-0.882706
C	0.072433	2.299648	-1.051511
C	3.337248	0.900772	-1.672307
C	3.114025	-1.675104	-1.380887
H	-3.467722	-0.579185	2.125462
C	-4.521822	-2.395997	1.537683
C	-6.418113	-1.014874	0.645204
C	-6.517927	-1.936180	-0.587101
C	-4.608789	-3.314957	0.301494
C	2.865369	-2.422831	-0.041999
C	2.454150	-2.474119	-2.546786
C	2.500247	1.990073	-1.577246
C	0.288840	3.772938	-1.274627
H	4.379426	0.913245	-1.950752
C	4.648682	-1.666454	-1.635211
H	-4.149334	-2.968312	2.396764
C	-5.915695	-1.823263	1.856895
H	-7.404225	-0.587468	0.868441
H	-6.906340	-1.375001	-1.447600
H	-7.225869	-2.752382	-0.391867
H	-3.624346	-3.741444	0.078981
H	-5.288122	-4.153162	0.505823
H	3.344822	-1.869216	0.776182
C	3.416616	-3.861726	-0.109399
C	3.011661	-3.912706	-2.596544
H	2.657644	-1.955869	-3.493185
H	2.748963	3.023960	-1.766981
C	0.621913	4.639066	-0.219018
C	0.167543	4.356417	-2.548729
H	4.864733	-1.159051	-2.583547
H	5.154558	-1.099743	-0.842614
C	5.210546	-3.101497	-1.691907
H	-6.617733	-2.635389	2.086497
H	-5.867702	-1.180597	2.746316
C	2.726019	-4.625388	-1.258449
C	4.936611	-3.819364	-0.356297
H	3.208660	-4.364268	0.843732
C	4.532314	-3.872379	-2.842025
H	2.517568	-4.452985	-3.413915
C	0.823975	6.005604	-0.408719
C	0.364843	5.720635	-2.763691
H	6.292560	-3.048833	-1.869034
H	1.646133	-4.675462	-1.081339
H	3.098676	-5.657534	-1.297259
H	5.345535	-4.837815	-0.384816
H	5.441361	-3.294501	0.465903
H	4.750634	-3.387111	-3.802789
H	4.934990	-4.892078	-2.901036
H	1.079149	6.632165	0.438020
C	0.693306	6.541608	-1.687642
H	0.259844	6.124336	-3.764056
H	0.848323	7.604181	-1.846106
Cl	0.798138	4.008501	1.411704
Cl	-0.246271	3.360387	-3.931214
N	-0.001153	-0.969683	1.641726
C	0.196303	0.028486	2.678889
C	1.546596	-0.043882	3.404695
H	-0.629676	0.010185	3.405115
H	0.113268	0.985686	2.146835
C	1.709548	1.058613	4.457730
H	1.634512	-1.027582	3.884701
H	2.351826	0.017025	2.662223
C	3.043359	0.966311	5.223673
H	1.638002	2.042701	3.973515
H	0.882073	1.010190	5.177913
H	3.114963	-0.008803	5.721839

H	3.867264	1.007940	4.495683
N	-0.289411	-3.482716	2.075449
N	-0.115072	-2.417541	2.414948
C	3.215103	2.065507	6.236124
C	3.353252	1.886143	7.550071
H	3.211046	3.081913	5.838499
H	3.467276	2.722475	8.233596
H	3.361856	0.891856	7.991422

2 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.130011 a.u.

(U)M06-L/BS2 SCF energy: -3260.019812 a.u.

(U)M06-L/BS2 Free energy: -3259.294407 a.u.

Fe	0.305476	0.084765	-0.514835
Cl	1.062779	0.261097	-2.657147
N	-1.231774	1.371608	-0.205170
N	-0.633866	-1.696996	-0.244438
C	-0.269536	-3.003933	-0.333827
C	-1.301561	-3.823693	0.200523
H	-1.287295	-4.900956	0.258386
C	-2.316025	-2.993457	0.622335
C	-1.909416	-1.658863	0.345500
C	-1.394774	2.720127	-0.282617
C	0.996031	-3.532074	-0.986669
C	2.259727	-2.721579	-0.597431
H	2.141257	-1.676159	-0.893396
C	1.240548	-5.012137	-0.574796
H	1.340136	-5.083671	0.516225
H	0.378121	-5.625576	-0.860003
C	0.832897	-3.495950	-2.538975
H	-0.047773	-4.088350	-2.818947
H	0.651296	-2.468354	-2.866211
C	2.094131	-4.060557	-3.226420
H	1.954400	-4.011980	-4.313707
H	1.345502	2.408840	-0.798725
H	-0.286057	2.654182	-2.802606
C	-2.406214	0.840612	0.356100
H	-3.253329	-3.284161	1.073495
C	-2.682690	-0.514888	0.604446
C	-2.673606	3.074272	0.227259
C	-0.408249	3.704408	-0.887319
H	2.385861	-2.743920	0.493094
C	3.514353	-3.286631	-1.295616
C	2.498631	-5.579347	-1.263404
C	2.312879	-5.523679	-2.793321
C	3.322478	-3.218648	-2.824868
C	1.057678	3.412092	-0.474133
C	-0.510042	3.662793	-2.444465
C	-3.299384	1.913584	0.625613
C	-4.025837	-0.784147	1.229072
H	-3.075657	4.073638	0.287974
C	-0.745359	5.153961	-0.433435
H	4.383548	-2.681093	-1.006853
C	3.732088	-4.748367	-0.862379
H	2.634756	-6.620997	-0.945216
H	1.454532	-6.140070	-3.091979
H	3.195783	-5.940688	-3.295405
H	3.185471	-2.177937	-3.141306
H	4.220037	-3.597290	-3.331740
H	1.141063	3.441319	0.620358
C	2.025812	4.428517	-1.114425
C	0.464773	4.680479	-3.074133
H	-1.541391	3.893087	-2.741590
H	-4.285209	1.817413	1.056352
C	-4.198154	-0.816506	2.624007
C	-5.172205	-1.015257	0.447993
H	-1.767603	5.410313	-0.734556
H	-0.705656	5.219797	0.661620
C	0.224669	6.173433	-1.064728
H	4.633860	-5.155460	-1.338115
H	3.889646	-4.803874	0.223179
C	1.909553	4.344823	-2.650301
C	1.669914	5.850024	-0.640994
H	3.051413	4.182303	-0.809138
C	0.109495	6.103880	-2.600943

H	0.379025	4.620443	-4.166444
C	-5.437030	-1.063805	3.215146
C	-6.421203	-1.264073	1.017150
H	-0.046389	7.179099	-0.718456
H	2.178753	3.339141	-2.994076
H	2.611535	5.047830	-3.117954
H	2.364594	6.580449	-1.076061
H	1.770476	5.923748	0.450284
H	-0.909944	6.364480	-2.915071
H	0.783633	6.836989	-3.063064
H	-5.520604	-1.079053	4.295672
C	-6.547120	-1.287221	2.404061
H	-7.276658	-1.436027	0.374234
H	-7.515381	-1.480250	2.855236
Cl	-2.825286	-0.540897	3.681492
Cl	-5.058261	-0.994561	-1.301941
N	1.587993	0.303902	0.714689
C	2.906182	0.566639	1.134254
C	3.120541	0.575929	2.659834
H	3.227890	1.530447	0.695735
H	3.570154	-0.180606	0.658978
C	4.573736	0.872897	3.047016
H	2.450731	1.324155	3.101634
H	2.811271	-0.396709	3.061736
C	4.799621	0.890702	4.570889
H	5.240082	0.125200	2.596278
H	4.874628	1.842749	2.625720
H	4.115419	1.628816	5.015545
H	4.527088	-0.083398	4.995947
C	6.215291	1.231385	4.949147
C	7.040996	0.440023	5.634331
H	6.574064	2.206606	4.615175
H	8.056662	0.741950	5.872806
H	6.728741	-0.540389	5.987373

2’ (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.1282 a.u.

(U)M06-L/BS2 SCF energy: -3260.024261 a.u.

(U)M06-L/BS2 Free energy: -3259.298048 a.u.

Fe	-0.026116	0.014757	0.578866
Cl	0.026611	0.009664	2.839830
N	1.156867	1.539478	-0.034165
N	1.097394	-1.568324	-0.025800
C	0.936080	-2.919058	-0.083107
C	2.198809	-3.544029	-0.270235
H	2.374278	-4.604674	-0.356349
C	3.151485	-2.551176	-0.323209
C	2.472023	-1.311860	-0.177646
C	1.045472	2.896022	-0.099047
C	-0.382336	-3.668475	0.014526
C	-1.303780	-3.339626	-1.198249
H	-1.514374	-2.264647	-1.223237
C	-0.115872	-5.201318	0.001303
H	0.411416	-5.476349	-0.920337
H	0.537953	-5.468981	0.840685
C	-1.143721	-3.335858	1.327431
H	-0.507562	-3.569998	2.189421
H	-1.349985	-2.263299	1.385906
C	-2.464802	-4.131202	1.408144
H	-2.982620	-3.863602	2.337929
H	-1.435502	2.315075	-1.215353
H	-1.253873	2.335166	1.390554
C	2.520203	1.230551	-0.186704
H	4.215220	-2.672834	-0.465123
C	3.090187	-0.052790	-0.233749
C	2.328973	3.471078	-0.292624
C	-0.245064	3.691587	-0.000770
H	-0.775396	-3.582690	-2.129229
C	-2.620339	-4.143804	-1.109612
C	-1.429564	-6.000610	0.090659
C	-2.161094	-5.641795	1.398450
C	-3.359936	-3.793929	0.197426
C	-1.187541	3.382607	-1.202319
C	-1.008034	3.399050	1.321105
C	3.244327	2.441866	-0.341336

C	4.587503	-0.081429	-0.386197
H	2.543827	4.523836	-0.386064
C	0.074338	5.214270	-0.033264
H	-3.250829	-3.886756	-1.970706
C	-2.316544	-5.654605	-1.121477
H	-1.192784	-7.072208	0.081478
H	-1.540661	-5.909479	2.263514
H	-3.093014	-6.216060	1.481832
H	-3.630541	-2.732461	0.203744
H	-4.299639	-4.358550	0.258517
H	-0.659306	3.596159	-2.140530
C	-2.475209	4.231983	-1.112325
C	-2.298666	4.242345	1.404141
H	-0.357143	3.617421	2.176117
H	4.311538	2.522713	-0.486222
C	5.206723	-0.097440	-1.648221
C	5.438026	-0.094131	0.734065
H	0.743364	5.467874	0.798409
H	0.604304	5.460438	-0.961569
C	-1.210019	6.059129	0.057330
H	-3.252182	-6.227763	-1.083812
H	-1.807990	-5.933845	-2.053671
C	-3.215388	3.923519	0.204865
C	-2.118884	5.731083	-1.143738
H	-3.121247	3.987439	-1.965515
C	-1.941847	5.740935	1.375348
H	-2.817674	4.003013	2.340917
C	6.593489	-0.125204	-1.795870
C	6.827173	-0.121866	0.609558
H	-0.936499	7.121735	0.033644
H	-3.522839	2.872703	0.227522
H	-4.133778	4.522291	0.266325
H	-3.033690	6.336776	-1.104741
H	-1.608754	5.982309	-2.082961
H	-1.304169	5.995787	2.231754
H	-2.851782	6.349192	1.460852
H	7.025412	-0.137045	-2.789846
C	7.399695	-0.137404	-0.660001
H	7.442710	-0.131041	1.501622
H	8.479931	-0.159060	-0.764949
Cl	4.227104	-0.083046	-3.104541
Cl	4.755944	-0.075597	2.347269
N	-1.723196	0.017441	-0.016184
C	-3.071179	0.074203	0.409278
C	-4.107632	0.125869	-0.728281
H	-3.207413	0.922132	1.104100
H	-3.251461	-0.809931	1.048054
C	-5.551912	0.175221	-0.217025
H	-3.900189	1.005176	-1.350825
H	-3.963167	-0.749755	-1.373022
C	-6.586525	0.262473	-1.355338
H	-5.762960	-0.713573	0.392328
H	-5.675972	1.039538	0.450816
H	-6.356092	1.148289	-1.966086
H	-6.483715	-0.607232	-2.016403
C	-8.002817	0.355771	-0.856916
C	-8.972132	-0.520068	-1.122987
H	-8.225901	1.214405	-0.221091
H	-9.976960	-0.398959	-0.728990
H	-8.796946	-1.391195	-1.750640

TS2 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.094944 a.u.

(U)M06-L/BS2 SCF energy: -3259.984164 a.u.

(U)M06-L/BS2 Free energy: -3259.261793 a.u.

Fe	0.100946	-0.880283	-0.496319
Cl	0.258805	-2.772898	-1.734968
N	1.736569	0.414439	-0.411810
N	-1.358830	0.527909	-0.914399
C	-2.691984	0.457217	-1.175215
C	-3.239424	1.766947	-1.254546
H	-4.271383	2.012931	-1.452335
C	-2.210625	2.657283	-1.034458
C	-1.031699	1.888768	-0.822382
C	3.068283	0.253093	-0.224369

C	-3.477003	-0.826110	-1.384723
C	-3.216243	-1.861272	-0.255561
H	-2.153675	-2.121557	-0.220081
C	-5.002521	-0.527319	-1.404102
H	-5.301167	-0.052713	-0.460028
H	-5.228496	0.184552	-2.206865
C	-3.107588	-1.476270	-2.753939
H	-3.315468	-0.756367	-3.556090
H	-2.037661	-1.699004	-2.784326
C	-3.923096	-2.768651	-2.974778
H	-3.632831	-3.207357	-3.937592
H	2.117384	-2.302840	0.439856
H	2.832469	-1.822271	-2.038322
C	1.483428	1.795996	-0.391428
H	-2.271293	3.735840	-1.027606
C	0.244929	2.429830	-0.573040
C	3.697049	1.526633	-0.073686
C	3.806951	-1.074827	-0.226288
H	-3.488104	-1.414151	0.713079
C	-4.030120	-3.151329	-0.486803
C	-5.820590	-1.814473	-1.629467
C	-5.428422	-2.438748	-2.984120
C	-3.625122	-3.770898	-1.840736
C	3.154566	-2.113899	0.726270
C	3.849564	-1.664762	-1.669926
C	2.716647	2.482750	-0.174210
C	0.286409	3.933603	-0.499093
H	4.750145	1.698714	0.085947
C	5.276647	-0.869130	0.237378
H	-3.810278	-3.859356	0.322628
C	-5.533557	-2.816625	-0.494888
H	-6.887894	-1.558110	-1.635162
H	-5.659368	-1.741731	-3.800750
H	-6.016386	-3.348308	-3.164773
H	-2.559603	-4.026177	-1.833923
H	-4.183187	-4.702070	-2.006107
H	3.136568	-1.709281	1.747433
C	3.932547	-3.446269	0.696330
C	4.627568	-2.998023	-1.683653
H	4.331093	-0.938500	-2.338088
H	2.839301	3.554218	-0.113006
C	0.096446	4.621753	0.711236
C	0.515843	4.727192	-1.637719
H	5.777924	-0.155038	-0.427065
H	5.291180	-0.436456	1.246398
C	6.057866	-2.198220	0.222434
H	-6.124830	-3.730501	-0.637393
H	-5.833514	-2.389218	0.471751
C	3.938707	-4.006511	-0.741256
C	5.379922	-3.209309	1.166962
H	3.435719	-4.159198	1.366742
C	6.075751	-2.761843	-1.212636
H	4.630100	-3.393659	-2.707223
C	0.132193	6.012792	0.797554
C	0.556450	6.120474	-1.578084
H	7.085565	-2.008082	0.558449
H	2.912447	-4.194236	-1.076138
H	4.471814	-4.966497	-0.765186
H	5.937819	-4.154963	1.172319
H	5.386963	-2.827899	2.197175
H	6.585217	-2.060391	-1.886926
H	6.642435	-3.701891	-1.241805
H	-0.019697	6.495208	1.756088
C	0.364019	6.758929	-0.355526
H	0.737409	6.688356	-2.483285
H	0.394421	7.842587	-0.300636
Cl	-0.198157	3.725621	2.197070
Cl	0.763009	3.967762	-3.198261
N	-0.110350	-1.220900	1.379445
C	-0.520582	-0.445179	2.396735
C	-0.279650	-0.790060	3.854215
H	-1.356905	-1.198109	1.868349
H	-0.832407	0.598442	2.205929
C	-1.431469	-0.377600	4.782314
H	-0.059193	-1.859723	3.932253
H	0.636480	-0.252200	4.142946

C	-1.115748	-0.632665	6.268105
H	-1.659383	0.686832	4.635231
H	-2.341018	-0.928368	4.509698
H	-0.898215	-1.696912	6.421581
H	-0.198326	-0.083796	6.528428
C	-2.232365	-0.205710	7.181691
C	-2.910664	-1.016782	7.993548
H	-2.493277	0.853404	7.150505
H	-3.712071	-0.650776	8.628407
H	-2.685176	-2.079034	8.057044

3 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.12563 a.u.

(U)M06-L/BS2 SCF energy: -3260.020101 a.u.

(U)M06-L/BS2 Free energy: -3259.292882 a.u.

Fe	0.251722	-0.473432	-0.104860
Cl	1.118271	-1.905860	-1.610341
N	0.776808	1.484827	-0.367362
N	-1.796395	-0.253351	-0.250876
C	-2.854838	-1.111730	-0.260930
C	-4.055365	-0.395039	-0.004541
H	-5.046792	-0.818224	0.038391
C	-3.721087	0.930606	0.163618
C	-2.311341	1.029006	0.005968
C	1.959355	2.143590	-0.514453
C	-2.791873	-2.597378	-0.569253
C	-1.778065	-3.346879	0.339269
H	-0.777558	-2.920876	0.228868
C	-4.184579	-3.254537	-0.352561
H	-4.505977	-3.112970	0.687689
H	-4.929177	-2.763080	-0.990375
C	-2.403889	-2.814175	-2.064573
H	-3.144011	-2.308966	-2.699006
H	-1.434267	-2.355512	-2.269723
C	-2.358298	-4.320256	-2.397375
H	-2.066160	-4.439991	-3.448299
H	2.873292	-0.440515	0.055380
H	2.495770	0.266099	-2.463871
C	-0.209311	2.455721	-0.121502
H	-4.391665	1.753705	0.362825
C	-1.582216	2.228973	0.061076
C	1.747526	3.542487	-0.366302
C	3.297604	1.509305	-0.849088
H	-2.073534	-3.216678	1.389460
C	-1.733758	-4.848670	-0.013413
C	-4.148926	-4.759235	-0.690736
C	-3.748235	-4.943867	-2.168284
C	-1.324508	-5.020393	-1.491116
C	3.645391	0.330612	0.099643
C	3.291910	1.001270	-2.324479
C	0.407810	3.737595	-0.118386
C	-2.401419	3.461592	0.335094
H	2.505283	4.306453	-0.441536
C	4.438359	2.559896	-0.725376
H	-0.996157	-5.341624	0.632760
C	-3.124514	-5.470533	0.214140
H	-5.147945	-5.181636	-0.522184
H	-4.490435	-4.468346	-2.823281
H	-3.733852	-6.011573	-2.423829
H	-0.328454	-4.595271	-1.658089
H	-1.268946	-6.088274	-1.740814
H	3.668200	0.695499	1.135036
C	5.004589	-0.294747	-0.277884
C	4.656929	0.377289	-2.683550
H	3.075475	1.846993	-2.990444
H	-0.098904	4.679195	0.034852
C	-2.621359	3.927854	1.642685
C	-2.986659	4.208014	-0.703457
H	4.242304	3.403478	-1.398202
H	4.466214	2.959742	0.296650
C	5.804448	1.941937	-1.087094
H	-3.101455	-6.544390	-0.013241
H	-3.417381	-5.372930	1.268212
C	4.952010	-0.802631	-1.734007
C	6.112427	0.766345	-0.140305

H	5.202738	-1.134307	0.399145
C	5.766191	1.437458	-2.543665
H	4.617012	0.015825	-3.718994
C	-3.378312	5.067746	1.911661
C	-3.747333	5.351573	-0.459389
H	6.577905	2.714081	-0.983602
H	4.177241	-1.570691	-1.836657
H	5.909814	-1.268243	-2.001706
H	7.089809	0.330124	-0.385196
H	6.172275	1.121711	0.897372
H	5.579731	2.275735	-3.228426
H	6.738646	1.009219	-2.820343
H	-3.519498	5.387460	2.937551
C	-3.940174	5.776929	0.852713
H	-4.178122	5.894524	-1.292639
H	-4.530901	6.665702	1.051168
Cl	-1.931378	3.066692	3.010479
Cl	-2.767251	3.710218	-2.370434
C	0.020553	-1.004983	2.905228
C	2.524594	-3.118460	2.844014
C	1.009514	-1.356457	4.037976
H	-0.824284	-1.718652	2.905106
H	-0.433754	-0.019520	3.130118
C	1.537482	-2.799974	3.988926
H	1.834214	-0.635323	4.026099
H	0.476461	-1.210246	4.986094
H	2.027646	-3.026002	4.944115
H	0.679896	-3.482893	3.914766
N	0.570511	-0.861889	1.614328
H	2.695991	-4.201386	2.818328
C	3.847202	-2.411932	2.971842
C	5.025118	-3.018841	3.129766
H	3.820044	-1.323162	2.934481
H	5.950410	-2.457623	3.223710
H	5.107648	-4.103115	3.166044
H	2.062325	-2.849714	1.883601

TS3 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.112462 a.u.

(U)M06-L/BS2 SCF energy: -3260.011649 a.u.

(U)M06-L/BS2 Free energy: -3259.285707 a.u.

Fe	0.166701	-0.560257	-0.052521
Cl	0.719016	-2.300214	-1.394494
N	1.249540	1.181071	-0.304105
N	-1.716499	0.232920	-0.286508
C	-2.974021	-0.292092	-0.341224
C	-3.932662	0.741011	-0.165292
H	-5.004316	0.616830	-0.169706
C	-3.244418	1.924465	-0.005489
C	-1.859599	1.616265	-0.085932
C	2.570314	1.483951	-0.406603
C	-3.317953	-1.744138	-0.623465
C	-2.617911	-2.719749	0.362797
H	-1.533328	-2.599513	0.311329
C	-4.851157	-1.970405	-0.490874
H	-5.180186	-1.709474	0.523567
H	-5.384634	-1.308214	-1.183541
C	-2.916242	-2.113629	-2.083921
H	-3.436784	-1.439751	-2.776994
H	-1.843844	-1.960692	-2.225981
C	-3.285230	-3.580123	-2.391757
H	-2.976160	-3.813628	-3.418393
H	2.734224	-1.210279	0.332788
H	2.629443	-0.592922	-2.229391
C	0.562908	2.395428	-0.132371
H	-3.663522	2.909601	0.138470
C	-0.824652	2.566751	-0.021749
C	2.751851	2.893165	-0.298799
C	3.693982	0.493432	-0.654367
H	-2.923081	-2.473048	1.389039
C	-2.985511	-4.182849	0.037442
C	-5.226866	-3.432694	-0.803275
C	-4.807423	-3.772907	-2.247445
C	-2.554247	-4.515729	-1.406421
C	3.683649	-0.672028	0.372148

C	3.589955	-0.089621	-2.097238
C	1.511049	3.458686	-0.124409
C	-1.278501	3.990654	0.163446
H	3.694651	3.414792	-0.351078
C	5.072093	1.205863	-0.541079
H	-2.460846	-4.844476	0.739464
C	-4.506973	-4.375512	0.180178
H	-6.313423	-3.547591	-0.697246
H	-5.341152	-3.126490	-2.956877
H	-5.085039	-4.807931	-2.486808
H	-1.470030	-4.399473	-1.512192
H	-2.794779	-5.562645	-1.635090
H	3.773102	-0.260961	1.386301
C	4.837090	-1.657214	0.090109
C	4.744541	-1.078970	-2.361781
H	3.628131	0.736641	-2.819373
H	1.279189	4.508166	-0.016741
C	-1.423685	4.564447	1.438171
C	-1.577973	4.819195	-0.933312
H	5.125566	2.028159	-1.264951
H	5.181668	1.647047	0.458242
C	6.230548	0.225073	-0.811090
H	-4.779965	-5.418572	-0.027296
H	-4.823153	-4.161085	1.210153
C	4.688277	-2.229016	-1.335084
C	6.186175	-0.923803	0.214618
H	4.784971	-2.474004	0.820677
C	6.094851	-0.346928	-2.236460
H	4.634961	-1.485067	-3.375395
C	-1.840507	5.882708	1.621476
C	-1.995815	6.140703	-0.775491
H	7.180526	0.767482	-0.718910
H	3.738981	-2.768522	-1.426162
H	5.493292	-2.949087	-1.535212
H	7.016278	-1.620482	0.037778
H	6.311526	-0.527604	1.231432
H	6.158475	0.462990	-2.975532
H	6.922737	-1.037157	-2.446142
H	-1.936932	6.279208	2.625548
C	-2.125456	6.667846	0.507067
H	-2.213960	6.740214	-1.651705
H	-2.450034	7.695251	0.638886
Cl	-1.075718	3.614804	2.874876
Cl	-1.427230	4.198603	-2.566441
C	-0.323086	-0.508389	2.909135
C	0.726959	-3.271706	2.802448
H	0.629998	-2.285561	2.027817
C	0.208399	-1.211380	4.174123
H	-1.420843	-0.619621	2.869671
H	-0.113942	0.569645	2.980569
C	0.014854	-2.732159	4.044180
H	1.271622	-0.973930	4.301651
H	-0.320168	-0.826211	5.053245
H	0.382241	-3.237530	4.946949
H	-1.057342	-2.949266	3.973297
N	0.299562	-1.001328	1.705751
H	0.179594	-4.053093	2.268262
C	2.166485	-3.559902	2.917216
C	2.809716	-4.520660	2.234596
H	2.735616	-2.931411	3.603020
H	3.874895	-4.689884	2.357448
H	2.287319	-5.165333	1.532355

4 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.147469 a.u.

(U)M06-L/BS2 SCF energy: -3260.03752 a.u.

(U)M06-L/BS2 Free energy: -3259.308917 a.u.

Fe	-0.166779	-0.593981	-0.162175
Cl	-0.779530	-2.225535	-1.589587
N	-1.063654	1.257133	-0.394743
N	1.802004	0.036807	-0.241945
C	3.005942	-0.598706	-0.237465
C	4.048038	0.345816	-0.020901
H	5.102734	0.124800	0.027816
C	3.464770	1.585779	0.104359

C	2.060820	1.403099	-0.038946
C	-2.347449	1.683514	-0.548345
C	3.235603	-2.079193	-0.493295
C	2.360263	-2.982994	0.416240
H	1.301577	-2.766699	0.259231
C	4.723002	-2.442941	-0.221972
H	4.980677	-2.204868	0.818288
H	5.375578	-1.838262	-0.863045
C	2.936225	-2.416172	-1.986420
H	3.574351	-1.793962	-2.627525
H	1.898170	-2.168659	-2.222951
C	3.200336	-3.911573	-2.265441
H	2.969537	-4.119826	-3.317836
H	-2.763800	-1.004534	0.097801
H	-2.531293	-0.320486	-2.440993
C	-0.276897	2.401749	-0.182827
H	3.963967	2.529422	0.268937
C	1.116947	2.442953	-0.012857
C	-2.402913	3.099880	-0.429023
C	-3.546033	0.802986	-0.859126
H	2.579950	-2.758454	1.468490
C	2.623055	-4.475036	0.121737
C	4.992455	-3.934970	-0.502230
C	4.679051	-4.240370	-1.980719
C	2.300375	-4.774409	-1.357204
C	-3.667270	-0.391075	0.125714
C	-3.449637	0.258883	-2.317845
C	-1.121445	3.546818	-0.199338
C	1.691984	3.817421	0.205754
H	-3.290757	3.707332	-0.510126
C	-4.862038	1.626613	-0.758182
H	1.976923	-5.081728	0.769168
C	4.100993	-4.803375	0.405680
H	6.049625	-4.147362	-0.296781
H	5.332500	-3.647710	-2.634741
H	4.881385	-5.297287	-2.198702
H	1.244766	-4.564302	-1.562703
H	2.467065	-5.839388	-1.567472
H	-3.756635	-0.004455	1.149778
C	-4.888567	-1.266548	-0.222159
C	-4.676004	-0.618533	-2.647942
H	-3.394103	1.108501	-3.011073
H	-0.799049	4.569322	-0.067789
C	1.841622	4.363169	1.492325
C	2.112823	4.622647	-0.868192
H	-4.824507	2.471981	-1.455737
H	-4.961902	2.045508	0.251696
C	-6.091006	0.756376	-1.091453
H	4.296490	-5.867961	0.221352
H	4.336943	-4.613100	1.461445
C	-4.745551	-1.802758	-1.661574
C	-6.173711	-0.425483	-0.106413
H	-4.933226	-2.109317	0.480660
C	-5.963262	0.220586	-2.531457
H	-4.572022	-0.999092	-3.671883
C	2.376943	5.632774	1.707918
C	2.651018	5.895474	-0.677935
H	-6.994294	1.374059	-1.005051
H	-3.842293	-2.417143	-1.747100
H	-5.601811	-2.444866	-1.907448
H	-7.053750	-1.042643	-0.329956
H	-6.294786	-0.054758	0.920395
H	-5.939392	1.055296	-3.244606
H	-6.839467	-0.390707	-2.784793
H	2.472458	6.008833	2.719906
C	2.780986	6.396037	0.615222
H	2.961169	6.478195	-1.537576
H	3.199202	7.385315	0.772401
Cl	1.348140	3.438264	2.902170
Cl	1.968529	4.032988	-2.513471
C	-0.125706	-0.515656	2.850974
C	-2.511197	-2.554912	3.527401
H	-0.833165	-2.126658	1.780660
C	-1.324342	-0.290821	3.796019
H	0.648352	-1.085774	3.392896
H	0.315346	0.456315	2.607448

C	-1.874575	-1.571448	4.462108
H	-2.122485	0.214374	3.238906
H	-1.004692	0.399912	4.587107
H	-2.620626	-1.254124	5.208457
H	-1.070128	-2.062751	5.025678
N	-0.462828	-1.192444	1.610390
C	-2.159034	-3.898665	3.432245
C	-2.753253	-4.824950	2.591841
H	-1.346586	-4.245989	4.072966
H	-2.423627	-5.857326	2.564952
H	-3.568667	-4.544794	1.931250
H	-3.329617	-2.190212	2.906285

TS4 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.144902 a.u.

(U)M06-L/BS2 SCF energy: -3260.038609 a.u.

(U)M06-L/BS2 Free energy: -3259.309251 a.u.

Fe	-0.145436	-0.671622	0.127379
Cl	-0.616706	-2.708631	-0.764440
N	-1.206306	1.019992	-0.377664
N	1.769061	0.158838	-0.217036
C	3.034204	-0.324920	-0.247443
C	3.972333	0.742361	-0.099794
H	5.046783	0.644838	-0.095579
C	3.254132	1.906944	0.011417
C	1.873274	1.553297	-0.072204
C	-2.521372	1.283226	-0.625973
C	3.420832	-1.775765	-0.479566
C	2.852710	-2.718731	0.618798
H	1.762848	-2.648554	0.644778
C	4.968294	-1.929970	-0.469456
H	5.368997	-1.601704	0.498503
H	5.409837	-1.282637	-1.237308
C	2.910729	-2.250238	-1.873200
H	3.334350	-1.597719	-2.648098
H	1.823675	-2.152422	-1.925633
C	3.321022	-3.715646	-2.130541
H	2.935730	-4.023445	-3.110871
H	-2.778413	-1.313002	0.356520
H	-2.253452	-0.983818	-2.183411
C	-0.565897	2.262005	-0.232356
H	3.643082	2.908977	0.119197
C	0.818673	2.477110	-0.085957
C	-2.745079	2.684749	-0.609694
C	-3.579736	0.243592	-0.949384
H	3.227539	-2.397138	1.600133
C	3.261752	-4.182817	0.345147
C	5.384730	-3.390587	-0.734193
C	4.857471	-3.833495	-2.113464
C	2.725239	-4.621676	-1.033264
C	-3.731351	-0.803554	0.187235
C	-3.225639	-0.493064	-2.276230
C	-1.532974	3.294518	-0.361641
C	1.232155	3.924569	-0.013262
H	-3.689827	3.177540	-0.779783
C	-4.963483	0.923780	-1.145974
H	2.831695	-4.821619	1.127495
C	4.797408	-4.301121	0.361603
H	6.480616	-3.453528	-0.719299
H	5.295696	-3.208625	-2.903104
H	5.161844	-4.868436	-2.318325
H	1.631974	-4.562854	-1.048004
H	2.999252	-5.668317	-1.222795
H	-3.998566	-0.285127	1.118422
C	-4.811178	-1.847773	-0.170415
C	-4.309542	-1.536766	-2.620950
H	-3.142064	0.246970	-3.082880
H	-1.335252	4.354945	-0.303496
C	1.330369	4.621831	1.202609
C	1.540524	4.656279	-1.175984
H	-4.898310	1.667152	-1.949886
H	-5.247092	1.461117	-0.231598
C	-6.049045	-0.113567	-1.497883
H	5.100024	-5.342576	0.190110
H	5.191920	-4.011949	1.345258

C	-4.419152	-2.567268	-1.477836
C	-6.167872	-1.141958	-0.356245
H	-4.882736	-2.579131	0.645559
C	-5.667187	-0.832543	-2.807008
H	-4.025267	-2.047708	-3.549477
C	1.712208	5.961695	1.270970
C	1.923920	5.996598	-1.133881
H	-7.006555	0.407395	-1.627208
H	-3.464568	-3.088476	-1.349662
H	-5.174861	-3.324200	-1.727084
H	-6.948800	-1.877562	-0.589385
H	-6.467794	-0.640958	0.574212
H	-5.610968	-0.109425	-3.631675
H	-6.441438	-1.563480	-3.075355
H	1.773417	6.452223	2.235436
C	2.008731	6.645849	0.095232
H	2.150846	6.515835	-2.057756
H	2.306904	7.688749	0.136774
Cl	0.968700	3.807790	2.717453
Cl	1.446157	3.886432	-2.748662
C	0.039745	0.051160	3.101811
C	-2.113165	-1.981635	3.502749
H	0.149851	-1.880006	2.373687
C	-1.318892	0.414497	3.732641
H	0.723125	-0.301187	3.887255
H	0.477474	0.957880	2.669914
C	-1.957286	-0.808390	4.416572
H	-1.979900	0.787621	2.941821
H	-1.188081	1.228907	4.456308
H	-2.946731	-0.507884	4.796787
H	-1.362469	-1.095884	5.293436
N	-0.112931	-0.950452	2.058745
C	-1.693266	-3.283097	3.827568
C	-1.889123	-4.390989	3.039850
H	-1.163465	-3.411834	4.772942
H	-1.532840	-5.369698	3.342239
H	-2.392537	-4.318769	2.080487
H	-2.706789	-1.842938	2.603853

5 (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.213808 a.u.

(U)M06-L/BS2 SCF energy: -3260.095997 a.u.

(U)M06-L/BS2 Free energy: -3259.36088 a.u.

Fe	0.024997	-0.689573	-0.112086
Cl	0.292963	-2.635498	-1.291038
N	-1.618483	0.528795	-0.296632
N	1.528011	0.784658	-0.243074
C	-2.955987	0.314721	-0.426037
C	-3.653514	1.551149	-0.377231
H	-4.722068	1.682145	-0.453510
C	-2.712353	2.547534	-0.224252
H	-2.894022	3.610516	-0.160777
C	-1.438466	1.916005	-0.183428
C	-0.209505	2.600113	-0.090335
C	-0.336262	4.099638	0.000254
C	-0.375220	4.905641	-1.152796
C	-0.496521	6.293764	-1.088642
H	-0.522318	6.870176	-2.006105
C	-0.582151	6.916298	0.154128
C	-0.546960	6.158427	1.321812
H	-0.612341	6.627735	2.296538
C	-0.425853	4.772034	1.230652
C	1.110213	2.121824	-0.110423
C	2.264715	2.961057	-0.039347
H	2.258746	4.035801	0.068563
C	3.361975	2.143462	-0.146718
H	4.396728	2.449507	-0.141548
C	2.881399	0.804507	-0.279454
C	-3.603429	-1.039166	-0.652039
C	-5.147486	-0.931907	-0.508729
H	-5.403020	-0.556098	0.490926
H	-5.535966	-0.206317	-1.233338
C	-3.108235	-2.097260	0.369001
H	-2.023417	-2.214386	0.282862
H	-3.328357	-1.747445	1.386997

C	-5.824592	-2.295218	-0.749639
H	-6.909981	-2.176734	-0.635916
C	-3.296300	-1.554487	-2.092558
H	-3.659195	-0.816789	-2.820092
H	-2.214938	-1.644819	-2.231128
C	-3.779071	-3.464075	0.118754
H	-3.397080	-4.188346	0.850473
C	-5.305045	-3.321492	0.275971
H	-5.794160	-4.292145	0.121636
H	-5.554297	-2.996361	1.295361
C	-5.501231	-2.780268	-2.177431
H	-5.895012	-2.068230	-2.914938
H	-5.992276	-3.743491	-2.369271
C	-3.974258	-2.920064	-2.332773
H	-3.734019	-3.259413	-3.348218
C	-3.445977	-3.945575	-1.308692
H	-2.363005	-4.065691	-1.422677
H	-3.905893	-4.926684	-1.487773
C	3.586663	-0.937367	-1.962487
H	2.543428	-1.221938	-2.122794
H	3.818779	-0.130126	-2.669573
C	3.772967	-0.404323	-0.509052
C	5.268820	-0.014881	-0.341293
H	5.440610	0.380032	0.668877
H	5.523190	0.784759	-1.047260
C	3.471391	-1.554601	0.488382
H	3.617512	-1.190834	1.516354
H	2.431396	-1.875989	0.390572
C	4.507506	-2.149704	-2.216262
H	4.344836	-2.507947	-3.240622
C	5.979927	-1.731930	-2.037134
H	6.242213	-0.944836	-2.756749
H	6.644045	-2.582956	-2.238198
C	6.191771	-1.223148	-0.597025
H	7.234503	-0.905858	-0.465853
C	4.389838	-2.765775	0.223980
H	4.137746	-3.560223	0.937645
C	4.167103	-3.273828	-1.216033
H	4.803755	-4.148879	-1.403972
H	3.126586	-3.590158	-1.346508
C	5.861179	-2.347630	0.403400
H	6.522546	-3.208337	0.237301
H	6.037789	-2.003310	1.431749
N	0.184667	-1.069601	2.075033
H	1.185757	-0.926053	2.202085
C	-0.531150	-0.061913	2.922186
H	-1.486390	0.176003	2.445856
H	0.053631	0.858627	2.972403
C	-0.758477	-0.755300	4.266434
H	0.155678	-0.729485	4.872370
H	-1.558581	-0.291659	4.850480
C	-1.084976	-2.191054	3.829966
H	-2.130027	-2.254031	3.508660
H	-0.937549	-2.932223	4.619936
C	-0.146614	-2.452975	2.618999
H	-0.658350	-3.014994	1.835459
C	1.100411	-3.197908	3.011722
H	1.657991	-2.786499	3.855768
C	1.521016	-4.316696	2.420397
H	0.990499	-4.743045	1.573043
H	2.411740	-4.838110	2.757844
H	-0.676424	7.996082	0.213112
Cl	-0.385135	3.864373	2.736778
Cl	-0.270408	4.169667	-2.740829

TS3' (quintuplet)

(U)B3LYP/BS1 SCF energy: -3260.111757 a.u.

(U)M06-L/BS2 SCF energy: -3260.009742 a.u.

(U)M06-L/BS2 Free energy: -3259.284185 a.u.

Fe	0.147602	-0.807340	0.039267
Cl	0.379252	-2.741214	-1.102616
N	1.677114	0.573191	-0.272466
N	-1.439072	0.390854	-0.477256
C	-2.776804	0.193092	-0.637960
C	-3.447666	1.445424	-0.663970

H	-4.509777	1.592394	-0.783245
C	-2.494368	2.430405	-0.524713
C	-1.234252	1.780309	-0.419409
C	3.035575	0.536870	-0.273015
C	-3.459742	-1.151098	-0.823299
C	-3.142311	-2.133490	0.338099
H	-2.064802	-2.295760	0.416804
C	-5.003012	-0.965879	-0.868233
H	-5.348948	-0.499798	0.063593
H	-5.271238	-0.287467	-1.687351
C	-3.029869	-1.799280	-2.175251
H	-3.285241	-1.115128	-2.995280
H	-1.946377	-1.938148	-2.195195
C	-3.741355	-3.154449	-2.374043
H	-3.406073	-3.592444	-3.322704
H	2.449717	-2.042756	0.624323
H	2.737201	-1.629961	-1.950443
C	1.306623	1.929279	-0.289856
H	-2.655755	3.498476	-0.516996
C	0.002526	2.445678	-0.340834
C	3.556695	1.862708	-0.280841
C	3.893479	-0.714918	-0.333391
H	-3.464700	-1.682199	1.285315
C	-3.852786	-3.485556	0.121635
C	-5.721204	-2.314238	-1.074867
C	-5.266773	-2.939354	-2.409345
C	-3.385050	-4.104759	-1.212019
C	3.496295	-1.756700	0.746260
C	3.778544	-1.370190	-1.744443
C	2.487234	2.726516	-0.288928
C	-0.084601	3.949688	-0.364702
H	4.601286	2.132024	-0.286529
C	5.390959	-0.357769	-0.107043
H	-3.593854	-4.158070	0.950009
C	-5.377195	-3.267714	0.085629
H	-6.804342	-2.137046	-1.099579
H	-5.538054	-2.281744	-3.245967
H	-5.782140	-3.895070	-2.573158
H	-2.303390	-4.279162	-1.187084
H	-3.869032	-5.079016	-1.363414
H	3.596118	-1.301529	1.740851
C	4.380121	-3.017553	0.644382
C	4.665800	-2.630031	-1.829059
H	4.087480	-0.638349	-2.502387
H	2.518711	3.806062	-0.305736
C	-0.135381	4.714088	0.813296
C	-0.119077	4.666916	-1.574982
H	5.719715	0.363667	-0.864632
H	5.514630	0.123278	0.872081
C	6.281915	-1.613146	-0.194866
H	-5.896694	-4.226155	-0.044753
H	-5.722591	-2.843262	1.038138
C	4.224449	-3.646635	-0.755817
C	5.853245	-2.632824	0.877851
H	4.059180	-3.737240	1.408734
C	6.139371	-2.244727	-1.594141
H	4.552775	-3.075149	-2.825754
C	-0.222906	6.105929	0.800988
C	-0.205585	6.058652	-1.613521
H	7.325655	-1.316995	-0.027457
H	3.182597	-3.941958	-0.922977
H	4.836693	-4.555685	-0.826027
H	6.491757	-3.524602	0.828618
H	5.979652	-2.202857	1.880674
H	6.474336	-1.536661	-2.363854
H	6.781964	-3.131498	-1.674371
H	-0.260531	6.648624	1.738363
C	-0.258743	6.774425	-0.420059
H	-0.229541	6.565539	-2.571190
H	-0.326607	7.857570	-0.441530
Cl	-0.081828	3.919368	2.379619
Cl	-0.046235	3.811657	-3.103866
C	0.453538	-2.315112	2.675318
C	-0.958271	0.040357	3.767533
H	-0.529257	-0.348348	2.654840
C	-0.433058	-2.424182	3.932806

H	1.501964	-2.182373	2.993799
H	0.403867	-3.259753	2.113298
C	-0.447670	-1.077839	4.676490
H	-1.450498	-2.706894	3.637077
H	-0.047712	-3.220894	4.578933
H	-1.068291	-1.151753	5.579164
H	0.570376	-0.843554	5.008959
N	0.037672	-1.256191	1.792730
H	-0.448194	0.999110	3.895705
C	-2.417625	0.181668	3.625070
C	-3.055369	1.336387	3.375120
H	-3.004410	-0.732562	3.718666
H	-4.135118	1.376653	3.271205
H	-2.514561	2.271798	3.261921

L ($CH_3CH_2OCH_2CH_3$)

B3LYP/BS1 SCF energy: -233.6728286 a.u.

M06-L/BS2 SCF energy: -233.6414067 a.u.

M06-L/BS2 Free energy: -233.5346477 a.u.

C	-2.378562	0.416451	0.000036
C	-1.183126	-0.522082	0.000098
H	-3.313723	-0.152152	0.000138
H	-2.361728	1.057816	0.885840
H	-2.361798	1.057613	-0.885916
H	-1.207378	-1.178966	0.886557
H	-1.207443	-1.179163	-0.886214
C	1.183126	-0.522082	0.000014
H	1.207439	-1.178970	0.886469
H	1.207384	-1.179159	-0.886302
C	2.378561	0.416451	-0.000123
H	2.361786	1.057813	0.885685
H	3.313723	-0.152152	-0.000084
H	2.361739	1.057617	-0.886071
O	0.000000	0.257158	-0.000031

N_2

B3LYP/BS1 SCF energy: -109.5207183 a.u.

M06-L/BS2 SCF energy: -109.5108891 a.u.

M06-L/BS2 Free energy: -109.5237371 a.u.

N	0.000000	0.000000	0.552613
N	0.000000	0.000000	-0.552613

1a

B3LYP/BS1 SCF energy: -399.435313 a.u.

M06-L/BS2 SCF energy: -399.4064362 a.u.

M06-L/BS2 Free energy: -399.2742302 a.u.

N	-2.782772	0.767755	-0.378368
C	-1.462096	0.972381	0.262907
C	-0.372616	0.052644	-0.298937
H	-1.545894	0.851115	1.351761
H	-1.213882	2.018547	0.068018
C	1.002272	0.331414	0.321164
H	-0.654193	-0.993703	-0.118787
H	-0.329378	0.182429	-1.387079
C	2.108361	-0.583471	-0.238865
H	1.283033	1.378270	0.146662
H	0.946510	0.206679	1.411591
H	1.811316	-1.630277	-0.076065
H	2.186420	-0.445980	-1.324535
N	-4.057897	-1.156406	0.177219
N	-3.391212	-0.254703	-0.047808
C	3.448031	-0.339151	0.400751
C	4.545066	0.061832	-0.241953
H	3.495591	-0.500204	1.479130
H	5.484586	0.226603	0.277335
H	4.544945	0.236111	-1.315736

1b

B3LYP/BS1 SCF energy: -635.837361 a.u.

M06-L/BS2 SCF energy: -635.781788 a.u.

M06-L/BS2 Free energy: -635.534687 a.u.

N	0.909931	-0.410536	0.121552

C	1.006345	-1.845519	0.419669
H	0.120799	-2.369823	0.058424
H	1.078174	-2.017875	1.502867
C	2.301683	-2.256496	-0.292656
H	2.752735	-3.156060	0.135909
H	2.095882	-2.453211	-1.351035
C	3.183867	-1.008532	-0.142200
H	3.990904	-0.946822	-0.876443
H	3.644547	-0.994182	0.852859
C	2.204374	0.185268	-0.276871
H	2.135981	0.521583	-1.318932
C	2.603358	1.353896	0.586371
H	2.621890	1.152996	1.658300
C	2.950864	2.552362	0.122631
H	2.919549	2.780282	-0.939739
H	3.264803	3.352766	0.785791
C	-0.251989	0.260767	-0.144084
O	-0.291884	1.374750	-0.645940
O	-1.328201	-0.481111	0.232625
C	-2.692845	0.029195	0.043429
C	-2.895779	1.304127	0.869848
C	-2.973740	0.253548	-1.446694
C	-3.553828	-1.113131	0.590144
H	-2.652112	1.116860	1.920551
H	-2.264502	2.111687	0.499003
H	-3.943846	1.616691	0.814318
H	-2.783209	-0.665153	-2.011123
H	-4.025430	0.524777	-1.586480
H	-2.346397	1.050957	-1.845127
H	-4.614616	-0.857213	0.510061
H	-3.376820	-2.034252	0.026792
H	-3.321037	-1.302270	1.642131

1c

B3LYP/BS1 SCF energy: -289.986728 a.u.

M06-L/BS2 SCF energy: -289.954915 a.u.

M06-L/BS2 Free energy: -289.824229 a.u.

N	-0.438531	-1.193251	-0.164414
H	-0.370887	-1.279671	-1.178724
C	-1.816106	-0.817348	0.186870
H	-1.978927	-1.064824	1.243542
H	-2.532366	-1.403647	-0.395845
C	-1.952371	0.718559	-0.024461
H	-2.467548	0.943005	-0.964033
H	-2.533054	1.185676	0.777220
C	-0.486997	1.226771	-0.062656
H	-0.293442	2.038697	0.644782
H	-0.233410	1.605274	-1.059836
C	0.376974	-0.033479	0.253261
H	0.508569	-0.107464	1.341828
C	1.728194	-0.015164	-0.399409
H	1.719770	0.017772	-1.491526
C	2.894492	-0.008032	0.244649
H	2.944805	-0.038058	1.330384
H	3.841084	0.028153	-0.286422

Boc_2O

B3LYP/BS1 SCF energy: -768.085453 a.u.

M06-L/BS2 SCF energy: -768.031881 a.u.

M06-L/BS2 Free energy: -767.799784 a.u.

C	1.163527	-0.158867	-0.220919
O	1.214329	-1.227687	-0.771855
O	2.151329	0.605600	0.229060
C	3.563493	0.189143	0.049236
C	3.812699	-1.116462	0.808553
C	3.880582	0.070807	-1.443693
C	4.326584	1.352281	0.684600
H	3.530783	-1.005900	1.860041
H	3.245708	-1.940952	0.375013
H	4.878335	-1.362802	0.765909
H	3.637772	1.004310	-1.960639
H	4.950597	-0.120251	-1.572392
H	3.323452	-0.746068	-1.903587
H	5.403075	1.167140	0.626365

H	4.105975	2.289361	0.165811
H	4.049902	1.466626	1.736353
O	0.000070	0.551587	0.001374
C	-1.163662	-0.159217	0.221785
O	-1.214827	-1.228706	0.771336
O	-2.151085	0.605792	-0.227999
C	-3.563426	0.189256	-0.049529
C	-3.812202	-1.115514	-0.810400
C	-3.881442	0.069337	1.443072
C	-4.326010	1.353139	-0.684122
H	-3.529330	-1.003911	-1.861519
H	-3.245751	-1.940571	-0.377227
H	-4.877926	-1.361685	-0.768955
H	-3.639367	1.002423	1.961110
H	-4.951460	-0.122313	1.570879
H	-3.324296	-0.747788	1.902507
H	-5.402569	1.168246	-0.626344
H	-4.105280	2.289698	-0.164449
H	-4.049011	1.468325	-1.735702

TS5

B3LYP/BS1 SCF energy: -1058.065624 a.u.

M06-L/BS2 SCF energy: -1057.985508 a.u.

M06-L/BS2 Free energy: -1057.596701 a.u.

C	0.856018	-0.569051	0.533656
O	0.810824	-1.070077	1.644961
O	1.848111	-0.781427	-0.399685
C	2.442015	-2.122340	-0.506336
C	3.383451	-2.369754	0.678598
C	1.351689	-3.196638	-0.595691
C	3.226088	-2.040117	-1.818665
H	4.149653	-1.588831	0.725784
H	2.825660	-2.371053	1.615536
H	3.889267	-3.334375	0.560794
H	0.659476	-2.973568	-1.411872
H	1.812739	-4.171549	-0.785410
H	0.784524	-3.257244	0.335015
H	3.751060	-2.981831	-2.006751
H	2.552480	-1.842936	-2.657610
H	3.967356	-1.236163	-1.774906
O	-0.398217	-0.555481	-0.285308
C	-1.537463	-0.158295	0.293821
O	-1.633532	0.658751	1.198253
O	-2.550194	-0.769944	-0.325352
C	-3.952370	-0.455171	0.009265
C	-4.239149	-0.834168	1.465269
C	-4.241826	1.021319	-0.280104
C	-4.726666	-1.359970	-0.952311
H	-3.975602	-1.881216	1.642874
H	-3.673695	-0.206761	2.154501
H	-5.307668	-0.711824	1.670628
H	-3.975518	1.265082	-1.313374
H	-5.311127	1.216184	-0.148878
H	-3.682024	1.672337	0.391839
H	-5.802932	-1.224684	-0.809706
H	-4.479893	-1.120755	-1.990633
H	-4.481224	-2.410610	-0.773787
C	2.165036	1.550946	1.663457
C	1.244512	2.053865	-0.547165
H	0.128094	1.434158	1.150527
C	3.299452	2.026859	0.753170
H	2.373924	0.643344	2.234374
H	1.868877	2.339927	2.365063
C	2.549664	2.849875	-0.303962
H	1.396513	1.319004	-1.341216
H	4.054698	2.604050	1.293594
H	3.788302	1.165236	0.289509
H	2.310160	3.844243	0.093442
H	3.109368	2.992350	-1.232111
N	1.046991	1.268881	0.726218
C	0.059591	2.916786	-0.875727
C	-0.644736	2.825312	-2.003799
H	-0.200945	3.672879	-0.133301
H	-1.476766	3.491326	-2.211481
H	-0.411459	2.079798	-2.759754

6

B3LYP/BS1 SCF energy: -1058.064268 a.u.

M06-L/BS2 SCF energy: -1057.985369 a.u.

M06-L/BS2 Free energy: -1057.597222 a.u.

C	0.902294	-0.522696	0.539647
O	0.807299	-1.037529	1.645308
O	1.881967	-0.818653	-0.391542
C	2.419826	-2.182990	-0.453564
C	3.350697	-2.422433	0.741960
C	1.293068	-3.221284	-0.510798
C	3.210696	-2.175939	-1.764914
H	4.143885	-1.667061	0.762428
H	2.789909	-2.371570	1.675797
H	3.823483	-3.407225	0.659994
H	0.607823	-2.997624	-1.332228
H	1.722115	-4.215959	-0.672205
H	0.724824	-3.231662	0.420428
H	3.698327	-3.143572	-1.918738
H	2.547909	-1.981493	-2.613126
H	3.983676	-1.401098	-1.745609
O	-0.416208	-0.587173	-0.349390
C	-1.537532	-0.148175	0.196778
O	-2.577881	-0.788929	-0.351107
O	-1.622106	0.739402	1.046235
C	2.093230	1.520368	1.645677
C	1.301692	1.886472	-0.660927
H	0.084135	1.352863	0.993436
C	2.914509	2.633805	0.984045
H	2.687059	0.624959	1.835810
H	1.619819	1.812764	2.583902
C	2.769969	2.333502	-0.515184
H	1.172480	1.163801	-1.465782
H	2.497811	3.618716	1.222985
H	3.953958	2.628307	1.323142
H	3.000924	3.187873	-1.156309
H	3.421005	1.501195	-0.798078
N	1.036823	1.151628	0.642170
C	0.339034	3.029781	-0.840501
C	-0.529364	3.108912	-1.848521
H	0.384507	3.831578	-0.102885
H	-1.197135	3.957555	-1.961148
H	-0.603046	2.323400	-2.596608
C	-3.965516	-0.447320	0.006879
C	-4.207711	-0.734205	1.492263
C	-4.264533	1.009198	-0.363756
C	-4.774194	-1.406326	-0.870805
H	-3.944458	-1.770467	1.725346
H	-3.615115	-0.070635	2.122319
H	-5.268062	-0.590887	1.725320
H	-4.036254	1.185754	-1.419747
H	-5.328379	1.215648	-0.207343
H	-3.679362	1.698369	0.245427
H	-5.844857	-1.263535	-0.696081
H	-4.567167	-1.227663	-1.929916
H	-4.519131	-2.444696	-0.641430

TS6

B3LYP/BS1 SCF energy: -1058.064234 a.u.

M06-L/BS2 SCF energy: -1057.985544 a.u.

M06-L/BS2 Free energy: -1057.596402 a.u.

C	-0.966741	-0.493721	-0.560419
O	-0.854167	-1.023566	-1.654984
O	-1.929797	-0.790693	0.376071
C	-2.468105	-2.156582	0.447296
C	-3.403767	-2.396744	-0.743981
C	-1.341606	-3.194412	0.504078
C	-3.253285	-2.141362	1.761724
H	-4.194893	-1.639292	-0.764735
H	-2.846716	-2.352856	-1.680428
H	-3.878807	-3.379789	-0.655885
H	-0.649294	-2.963701	1.317128
H	-1.771900	-4.186626	0.677092
H	-0.780287	-3.212858	-0.430956

H	-3.741874	-3.107464	1.921421
H	-2.586327	-1.945248	2.606219
H	-4.024995	-1.365256	1.742535
O	0.416455	-0.610121	0.375233
C	1.527789	-0.170699	-0.162049
O	2.582363	-0.819078	0.357011
O	1.612950	0.734351	-1.002794
C	-2.027995	1.575063	-1.665489
C	-1.271876	1.870301	0.666475
H	-0.035220	1.296013	-0.966636
C	-2.817560	2.708543	-0.999016
H	-2.655075	0.712746	-1.894991
H	-1.512835	1.867465	-2.581318
C	-2.717291	2.377660	0.497193
H	-1.184471	1.136253	1.465663
H	-2.359065	3.680416	-1.212483
H	-3.848846	2.748684	-1.359811
H	-2.927210	3.230187	1.147734
H	-3.407182	1.567916	0.752673
N	-1.013606	1.134143	-0.641524
C	-0.267149	2.972611	0.869991
C	0.562076	3.025902	1.911896
H	-0.250134	3.768929	0.125409
H	1.258158	3.848380	2.044895
H	0.575432	2.244190	2.667247
C	3.962000	-0.475716	-0.021259
C	4.178141	-0.740931	-1.514921
C	4.273794	0.974287	0.365179
C	4.785362	-1.449320	0.826842
H	3.909893	-1.773634	-1.758234
H	3.573849	-0.068110	-2.123631
H	5.234173	-0.594663	-1.765593
H	4.064247	1.135715	1.427530
H	5.335522	1.179924	0.193406
H	3.679414	1.673554	-0.223114
H	5.853133	-1.306550	0.634806
H	4.598069	-1.286098	1.892151
H	4.523326	-2.483639	0.587043

1d

B3LYP/BS1 SCF energy: -422.264109 a.u.

M06-L/BS2 SCF energy: -422.237745 a.u.

M06-L/BS2 Free energy: -422.119061 a.u.

O	2.493985	0.917821	-0.000036
C	1.493665	0.240587	-0.000189
O	1.523850	-1.120719	-0.000063
O	0.270337	0.766100	-0.000576
C	-1.006210	0.018923	0.000028
C	-1.131833	-0.819201	-1.275631
C	-1.131334	-0.817962	1.276554
C	-2.032710	1.155651	-0.000332
H	-0.981212	-0.190350	-2.158349
H	-0.409460	-1.635843	-1.296216
H	-2.138019	-1.246633	-1.331936
H	-0.980306	-0.188262	2.158597
H	-2.137511	-1.245297	1.333707
H	-0.409000	-1.634630	1.297610
H	-3.047063	0.746039	0.000022
H	-1.909464	1.784139	0.885734
H	-1.909745	1.783299	-0.887033
H	2.466935	-1.346071	0.000686

TS1-2a

B3LYP/BS1 SCF energy: -3299.427284 a.u.

M06-L/BS2 SCF energy: -3299.322745 a.u.

M06-L/BS2 Free energy: -3298.569476 a.u.

Fe	-0.014039	-0.549464	-0.133829
Cl	0.081210	-2.263480	-1.604589
N	1.445645	0.897882	-0.359922
N	-1.661693	0.682949	-0.290865
C	-3.006125	0.475383	-0.343189
C	-3.689430	1.716082	-0.206313
H	-4.759317	1.853462	-0.216371
C	-2.738559	2.700579	-0.064978

C	-1.467077	2.063956	-0.121044
C	2.803126	0.876998	-0.461129
C	-3.696200	-0.859399	-0.565379
C	-3.185754	-1.954309	0.411027
H	-2.109926	-2.101081	0.293332
C	-5.229115	-0.712835	-0.343597
H	-5.425392	-0.356058	0.676003
H	-5.633574	0.039078	-1.031826
C	-3.483751	-1.341651	-2.034233
H	-3.873970	-0.577944	-2.719818
H	-2.416464	-1.449747	-2.241867
C	-4.206436	-2.685048	-2.268789
H	-4.025574	-3.006134	-3.302455
H	2.304514	-1.818404	0.107764
H	2.373718	-1.038357	-2.401157
C	1.072100	2.236204	-0.151313
H	-2.907466	3.760816	0.053666
C	-0.236458	2.736399	-0.047297
C	3.317432	2.194562	-0.306106
C	3.656993	-0.341094	-0.771018
H	-3.351329	-1.620944	1.444228
C	-3.909526	-3.292836	0.158561
C	-5.958027	-2.049943	-0.581984
C	-5.719530	-2.510712	-2.034156
C	-3.655918	-3.746498	-1.294008
C	3.356444	-1.533341	0.176934
C	3.426719	-0.790764	-2.247229
C	2.247222	3.037724	-0.111266
C	-0.336009	4.227270	0.140438
H	4.358189	2.475723	-0.344227
C	5.166038	0.006672	-0.622543
H	-3.511362	-4.044738	0.851929
C	-5.421162	-3.115372	0.392588
H	-7.032413	-1.900886	-0.412955
H	-6.130280	-1.772677	-2.736062
H	-6.244941	-3.456663	-2.220862
H	-2.582208	-3.889489	-1.459904
H	-4.146251	-4.712312	-1.476116
H	3.536364	-1.223974	1.215003
C	4.237455	-2.749145	-0.177324
C	4.311408	-2.009481	-2.584242
H	3.666328	0.046682	-2.915552
H	2.275173	4.108258	0.030169
C	-0.367612	4.816191	1.416205
C	-0.405191	5.106491	-0.955642
H	5.423214	0.833716	-1.295121
H	5.371016	0.347276	0.400898
C	6.054494	-1.207001	-0.961717
H	-5.945593	-4.067674	0.238268
H	-5.612189	-2.809798	1.430285
C	3.967060	-3.176000	-1.635048
C	5.722682	-2.375419	-0.013774
H	3.988578	-3.576866	0.500493
C	5.797515	-1.636083	-2.420324
H	4.116332	-2.310237	-3.621382
C	-0.463142	6.195110	1.601649
C	-0.501620	6.488878	-0.795857
H	7.106720	-0.918940	-0.840151
H	2.915729	-3.460609	-1.755867
H	4.574828	-4.055793	-1.885627
H	6.359954	-3.240042	-0.241528
H	5.930817	-2.090185	1.026365
H	6.061631	-0.819626	-3.105564
H	6.435614	-2.490933	-2.680420
H	-0.484168	6.600068	2.606755
C	-0.530430	7.028428	0.487824
H	-0.553002	7.125352	-1.671629
H	-0.605383	8.103108	0.620971
Cl	-0.286285	3.807442	2.852668
Cl	-0.373000	4.472089	-2.590053
C	1.210660	-1.871064	4.521060
C	1.413930	-3.098265	3.615733
C	0.234957	-3.394616	2.694290
C	1.164929	-0.509519	3.808688
C	-0.020904	-0.300887	2.844359
H	0.285910	-2.004449	5.101150

H	2.323104	-2.969847	3.013102
H	2.097061	-0.343778	3.254641
H	-0.069227	0.761886	2.569223
H	2.025447	-1.846083	5.255069
H	1.589983	-3.980396	4.248134
H	1.108650	0.276603	4.572910
H	-0.965582	-0.521392	3.372026
N	0.061305	-1.049193	1.612270
H	0.115055	-2.350972	1.998053
H	-0.720293	-3.433814	3.231197
C	0.392984	-4.505549	1.742720
C	-0.558625	-5.409500	1.458860
H	1.356433	-4.577817	1.238000
H	-0.391305	-6.205741	0.740498
H	-1.532964	-5.379480	1.940431

TS2-2a

B3LYP/BS1 SCF energy: -3299.422471 a.u.

M06-L/BS2 SCF energy: -3299.316479 a.u.

M06-L/BS2 Free energy: -3298.565259 a.u.

Fe	-0.379704	0.252391	-0.177490
Cl	-1.923524	1.128045	-1.592909
N	0.081829	-1.750882	-0.362615
N	1.543019	0.996580	-0.296463
C	2.087004	2.243125	-0.363075
C	3.480681	2.175675	-0.087713
H	4.164851	3.009761	-0.078399
C	3.792987	0.856280	0.151486
C	2.588497	0.111273	0.017363
C	-0.644145	-2.894231	-0.496592
C	1.347506	3.515858	-0.736681
C	0.103146	3.757958	0.162521
H	-0.588025	2.915584	0.089194
C	2.282206	4.748650	-0.578394
H	2.633175	4.818424	0.459445
H	3.169145	4.625093	-1.211642
C	0.898287	3.457920	-2.228838
H	1.783668	3.312688	-2.861606
H	0.240683	2.599832	-2.388116
C	0.170352	4.759515	-2.624675
H	-0.144308	4.682941	-3.673140
H	-2.715547	-1.107969	0.050057
H	-1.910241	-1.419775	-2.452494
C	1.392066	-2.135274	-0.029735
H	4.765062	0.446222	0.383021
C	2.496933	-1.285335	0.142098
C	0.182951	-4.023065	-0.240439
C	-2.099829	-2.972437	-0.920356
H	0.423707	3.822549	1.211172
C	-0.625307	5.053934	-0.251769
C	1.559726	6.051302	-0.976516
C	1.119563	5.960798	-2.451329
C	-1.069240	4.951894	-1.726056
C	-3.025372	-2.154966	0.023471
C	-2.260047	-2.451962	-2.380741
C	1.443810	-3.555217	0.053356
C	3.790139	-1.980170	0.477758
H	-0.126916	-5.055702	-0.282330
C	-2.595120	-4.446733	-0.895987
H	-1.507429	5.184187	0.389193
C	0.323097	6.254880	-0.079054
H	2.253001	6.892646	-0.848097
H	1.998174	5.846859	-3.100294
H	0.617236	6.889279	-2.753438
H	-1.760672	4.111875	-1.854191
H	-1.605860	5.864761	-2.017511
H	-2.925338	-2.541878	1.046578
C	-4.493706	-2.246140	-0.441197
C	-3.734457	-2.539884	-2.826800
H	-1.628015	-3.056757	-3.044395
H	2.321552	-4.140666	0.284939
C	4.182509	-2.217408	1.806336
C	4.672346	-2.424366	-0.523984
H	-1.971019	-5.058346	-1.559209
H	-2.491014	-4.858067	0.116558

C	-4.065833	-4.546043	-1.350444
H	-0.190373	7.187363	-0.347981
H	0.629519	6.349628	0.971516
C	-4.615310	-1.699569	-1.878902
C	-4.955927	-3.715276	-0.405851
H	-5.116677	-1.645632	0.234477
C	-4.197961	-4.008902	-2.789708
H	-3.817954	-2.149421	-3.848889
C	5.379493	-2.856013	2.129624
C	5.874888	-3.065148	-0.225620
H	-4.374044	-5.599152	-1.318660
H	-4.305245	-0.649350	-1.910430
H	-5.662755	-1.740942	-2.206494
H	-6.007288	-3.791044	-0.713174
H	-4.892974	-4.109513	0.617489
H	-3.592527	-4.615619	-3.476239
H	-5.239985	-4.088470	-3.126697
H	5.637652	-3.015031	3.170145
C	6.223859	-3.278224	1.105732
H	6.522010	-3.388993	-1.032483
H	7.158050	-3.775838	1.346477
Cl	3.151158	-1.702277	3.131990
Cl	4.274186	-2.178308	-2.214066
C	-0.374368	0.302564	2.850873
C	-2.804930	1.906249	2.498246
H	-1.918506	1.260171	1.742286
C	-1.439424	0.366798	3.961226
H	0.409460	1.052295	3.056522
H	0.115636	-0.680977	2.868092
C	-2.202858	1.703779	3.877651
H	-2.134689	-0.473021	3.843775
H	-0.960214	0.258419	4.940713
H	-2.994542	1.728675	4.639576
H	-1.511859	2.523582	4.106847
N	-0.952398	0.494605	1.538924
C	-4.138680	1.232502	2.192162
H	-4.117240	0.187065	2.520550
H	-4.290297	1.226349	1.105150
H	-2.740380	2.927646	2.113358
C	-5.285645	1.953464	2.859767
C	-6.052352	1.443588	3.825040
H	-5.466814	2.973135	2.517783
H	-6.861516	2.013597	4.272359
H	-5.907317	0.430571	4.193679

TS3-2a

B3LYP/BS1 SCF energy: -3299.408424 a.u.

M06-L/BS2 SCF energy: -3299.296481 a.u.

M06-L/BS2 Free energy: -3298.547822 a.u.

Fe	-0.224714	0.271232	-0.329266
Cl	-1.518829	1.038329	-2.023535
N	0.240920	-1.744769	-0.388429
N	1.682030	1.013261	-0.213859
C	2.225454	2.264316	-0.237234
C	3.587092	2.201390	0.159960
H	4.265772	3.037346	0.226908
C	3.879760	0.883029	0.436817
C	2.696070	0.133634	0.201628
C	-0.471680	-2.890096	-0.552602
C	1.511202	3.534850	-0.663531
C	0.182734	3.742370	0.114925
H	-0.487918	2.893667	-0.040398
C	2.409865	4.774730	-0.391031
H	2.658613	4.827023	0.676961
H	3.355181	4.674334	-0.938087
C	1.213609	3.505486	-2.193881
H	2.161006	3.392519	-2.737160
H	0.592776	2.640888	-2.438980
C	0.503721	4.804871	-2.629959
H	0.291351	4.746327	-3.704919
H	-2.559540	-1.041178	-0.369591
H	-1.529985	-1.566861	-2.731413
C	1.512447	-2.117213	0.080111
H	4.827824	0.478151	0.759378
C	2.592773	-1.262138	0.342862

C	0.326562	-4.012026	-0.186147
C	-1.883263	-2.987324	-1.103856
H	0.401510	3.786679	1.190639
C	-0.520474	5.038694	-0.338744
C	1.711018	6.076888	-0.831339
C	1.413959	6.014683	-2.342986
C	-0.818824	4.959990	-1.850486
C	-2.880504	-2.083904	-0.328010
C	-1.897420	-2.588667	-2.611812
C	1.553834	-3.535349	0.210222
C	3.841467	-1.944392	0.835209
H	0.019299	-5.045511	-0.223393
C	-2.402917	-4.449933	-1.005539
H	-1.461319	5.144948	0.217185
C	0.392002	6.246644	-0.053120
H	2.376954	6.923343	-0.619237
H	2.350971	5.928036	-2.909110
H	0.927578	6.943332	-2.669747
H	-1.479719	4.111464	-2.060297
H	-1.341532	5.869334	-2.176086
H	-2.882558	-2.374144	0.730997
C	-4.300406	-2.204181	-0.919167
C	-3.324445	-2.706278	-3.187346
H	-1.213302	-3.248630	-3.161313
H	2.403918	-4.112499	0.543341
C	4.086759	-2.135697	2.206074
C	4.823986	-2.424186	-0.049472
H	-1.732282	-5.119604	-1.557556
H	-2.396390	-4.777859	0.042234
C	-3.826188	-4.576135	-1.585109
H	-0.105632	7.178528	-0.352028
H	0.595286	6.323123	1.023638
C	-4.278649	-1.781752	-2.403157
C	-4.787650	-3.660787	-0.803040
H	-4.973626	-1.542603	-0.358390
C	-3.813086	-4.163012	-3.070952
H	-3.304547	-2.404427	-4.242208
C	5.237457	-2.766527	2.678063
C	5.983068	-3.058101	0.398578
H	-4.152381	-5.620338	-1.494141
H	-3.951930	-0.739836	-2.493982
H	-5.290976	-1.844064	-2.824652
H	-5.806600	-3.754270	-1.201252
H	-4.826761	-3.965798	0.251418
H	-3.154936	-4.831181	-3.642357
H	-4.819382	-4.262742	-3.498804
H	5.380669	-2.890609	3.745180
C	6.184364	-3.226885	1.766293
H	6.711580	-3.410852	-0.322195
H	7.083367	-3.719258	2.123578
Cl	2.921708	-1.571591	3.393733
Cl	4.613179	-2.232044	-1.779821
C	-0.688502	0.730700	2.671229
C	-2.043234	0.860211	3.397005
H	-0.084969	1.640047	2.826497
H	-0.085967	-0.121196	3.009118
C	-2.903089	1.608845	2.376133
H	-2.468345	-0.134817	3.571720
H	-1.967921	1.368481	4.365703
H	-2.675587	2.678552	2.314018
N	-1.047206	0.569703	1.266899
H	-2.200936	1.115961	1.347767
C	-4.367685	1.282671	2.222249
C	-5.225688	1.799284	3.410645
H	-4.502258	0.197714	2.136443
H	-4.749442	1.726795	1.294284
H	-5.066402	2.882668	3.508488
H	-4.880680	1.341116	4.344927
C	-6.690501	1.519340	3.215065
C	-7.436613	0.749024	4.007204
H	-7.149347	1.984791	2.341381
H	-8.491095	0.579066	3.810622
H	-7.020339	0.262455	4.886576

TS1-3a

B3LYP/BS1 SCF energy: -3338.733494 a.u.

M06-L/BS2 SCF energy: -3338.626698 a.u.

M06-L/BS2 Free energy: -3337.846194 a.u.

Fe	-0.043170	-0.518634	-0.177489
Cl	-0.002851	-2.231498	-1.653939
N	1.457756	0.894322	-0.410086
N	-1.653942	0.774553	-0.324115
C	-3.004693	0.616612	-0.392464
C	-3.646069	1.876721	-0.231115
H	-4.710369	2.051476	-0.246362
C	-2.663349	2.823634	-0.059008
C	-1.414415	2.144367	-0.120915
C	2.812714	0.840780	-0.538559
C	-3.741023	-0.685921	-0.650621
C	-3.296802	-1.813391	0.320965
H	-2.224901	-2.003299	0.226026
C	-5.271572	-0.480676	-0.460472
H	-5.476436	-0.131342	0.559951
H	-5.629623	0.296886	-1.145963
C	-3.515606	-1.155466	-2.121219
H	-3.859022	-0.366870	-2.803665
H	-2.449383	-1.304136	-2.307474
C	-4.286721	-2.464770	-2.391415
H	-4.095578	-2.778756	-3.425454
H	2.279159	-1.859557	-0.044258
H	2.261081	-0.987177	-2.529072
C	1.127976	2.234886	-0.146080
H	-2.796290	3.886098	0.082947
C	-0.163471	2.774424	-0.027769
C	3.368079	2.134874	-0.336261
C	3.625989	-0.381638	-0.929111
H	-3.472295	-1.487472	1.355004
C	-4.069230	-3.117299	0.033213
C	-6.048959	-1.783156	-0.734604
C	-5.796426	-2.232386	-2.187892
C	-3.802467	-3.560813	-1.419932
C	3.339831	-1.601069	-0.012832
C	3.325006	-0.769043	-2.409871
C	2.326426	2.999792	-0.090537
C	-0.215274	4.264731	0.184706
H	4.415784	2.387528	-0.381716
C	5.147543	-0.071635	-0.831005
H	-3.715843	-3.893112	0.723087
C	-5.577468	-2.882083	0.236260
H	-7.119910	-1.592175	-0.587188
H	-6.160837	-1.468088	-2.887318
H	-6.355024	-3.153444	-2.400875
H	-2.732198	-3.746375	-1.564098
H	-4.328349	-4.502786	-1.626647
H	3.574165	-1.331665	1.025670
C	4.175802	-2.822371	-0.449074
C	4.166641	-1.992968	-2.828544
H	3.556475	0.088070	-3.055815
H	2.387569	4.062779	0.091355
C	-0.238717	4.836580	1.468192
C	-0.245500	5.161663	-0.899100
H	5.395461	0.775795	-1.481354
H	5.401890	0.223638	0.195394
C	5.993223	-1.289947	-1.252786
H	-6.135728	-3.810589	0.057300
H	-5.779778	-2.582630	1.273616
C	3.835192	-3.186603	-1.909089
C	5.674719	-2.486271	-0.335419
H	3.935451	-3.668821	0.207510
C	5.666394	-1.657608	-2.713964
H	3.922178	-2.250383	-3.866908
C	-0.288707	6.215301	1.672836
C	-0.296426	6.544043	-0.720176
H	7.055870	-1.028970	-1.165296
H	2.773429	-3.443295	-1.996035
H	4.410765	-4.069574	-2.217689
H	6.282301	-3.354757	-0.621614
H	5.931769	-2.244123	0.704681
H	5.920742	-0.822065	-3.379638
H	6.273467	-2.515555	-3.031862
H	-0.304790	6.606306	2.683532

C	-0.317741	7.066199	0.570837
H	-0.319019	7.194127	-1.587150
H	-0.357212	8.140825	0.718783
Cl	-0.205578	3.806093	2.891107
Cl	-0.222431	4.550497	-2.542461
C	-0.058432	-0.211081	2.754470
C	1.565956	-3.420115	3.005723
C	1.057513	-0.363429	3.813124
C	1.715951	-2.841957	4.424098
C	0.910108	-1.573737	4.762319
H	-1.037137	-0.353927	3.245535
H	2.032116	-0.369134	3.310218
H	2.162632	-2.835059	2.296882
H	2.781461	-2.642761	4.597642
H	-0.053252	0.831680	2.406097
H	1.999319	-4.429659	3.000249
H	1.030274	0.552573	4.416301
H	1.432928	-3.614379	5.151515
H	1.212171	-1.268099	5.771452
H	-0.155716	-1.825349	4.847758
C	0.126827	-3.486871	2.491328
H	-0.625550	-3.539405	3.285414
N	0.040137	-1.033498	1.572948
H	-0.027608	-2.337116	1.976188
C	-0.146478	-4.443107	1.406037
C	-1.222724	-5.244794	1.355832
H	0.583578	-4.486514	0.598800
H	-1.378295	-5.938425	0.535530
H	-1.974216	-5.237065	2.141830

TS2-3a

B3LYP/BS1 SCF energy: -3338.737484 a.u.

M06-L/BS2 SCF energy: -3338.627015 a.u.

M06-L/BS2 Free energy: -3337.847909 a.u.

Fe	-0.355010	0.125433	-0.222014
Cl	-1.959962	0.482732	-1.784456
N	0.641722	-1.681613	-0.367246
N	1.279785	1.369845	-0.288038
C	1.445702	2.722834	-0.311945
C	2.801298	3.044378	-0.034388
H	3.219890	4.037812	0.007624
C	3.478710	1.859717	0.157307
C	2.536160	0.808102	-0.004835
C	0.260006	-2.980250	-0.491615
C	0.375451	3.742658	-0.660662
C	-0.907347	3.576090	0.199171
H	-1.321665	2.572945	0.076337
C	0.906853	5.185772	-0.427503
H	1.197384	5.310196	0.623886
H	1.805673	5.352012	-1.033301
C	0.001725	3.622191	-2.170283
H	0.907352	3.771114	-2.772906
H	-0.368241	2.616398	-2.383787
C	-1.066062	4.670389	-2.547803
H	-1.318359	4.550106	-3.608928
H	-2.209348	-1.761336	0.000481
H	-1.400078	-2.054113	-2.493537
C	2.021400	-1.684186	-0.099480
H	4.528935	1.736175	0.377597
C	2.845891	-0.561868	0.071513
C	1.384329	-3.834006	-0.300266
C	-1.134319	-3.470322	-0.844335
H	-0.646210	3.687337	1.260427
C	-1.972357	4.619867	-0.197174
C	-0.154862	6.237745	-0.808232
C	-0.513441	6.087227	-2.300159
C	-2.329155	4.453856	-1.689145
C	-2.224994	-2.850985	0.071006
C	-1.458228	-3.133077	-2.332616
C	2.474909	-3.033833	-0.053755
C	4.292761	-0.870796	0.351570
H	1.375101	-4.911818	-0.346211
C	-1.218259	-5.016261	-0.692090
H	-2.869309	4.460677	0.415873
C	-1.419585	6.036206	0.048763

H	0.259207	7.237975	-0.626366
H	0.374788	6.262554	-2.921702
H	-1.257659	6.841959	-2.586984
H	-2.738478	3.453630	-1.870411
H	-3.103372	5.180047	-1.970576
H	-2.005553	-3.103443	1.116784
C	-3.624666	-3.366415	-0.322580
C	-2.864226	-3.647291	-2.708619
H	-0.700865	-3.600233	-2.975821
H	3.491023	-3.350985	0.129396
C	4.778447	-1.036554	1.660003
C	5.231650	-1.008738	-0.686850
H	-0.473949	-5.494004	-1.340377
H	-0.979421	-5.302562	0.340484
C	-2.618937	-5.538355	-1.072360
H	-2.175148	6.789773	-0.209547
H	-1.181684	6.172358	1.112405
C	-3.917768	-2.993023	-1.790775
C	-3.677766	-4.896529	-0.155661
H	-4.371941	-2.898297	0.332143
C	-2.919361	-5.177987	-2.541053
H	-3.069623	-3.379723	-3.752821
C	6.116629	-1.322443	1.929565
C	6.574769	-1.294972	-0.442462
H	-2.634102	-6.628942	-0.948432
H	-3.898278	-1.904300	-1.913617
H	-4.923136	-3.335264	-2.070310
H	-4.677351	-5.272649	-0.410687
H	-3.489474	-5.172163	0.890759
H	-2.188733	-5.659201	-3.204824
H	-3.909334	-5.557019	-2.827368
H	6.442572	-1.441122	2.956379
C	7.012174	-1.450720	0.870650
H	7.260430	-1.392709	-1.276181
H	8.055736	-1.673399	1.069851
Cl	3.686738	-0.884487	3.028131
Cl	4.724922	-0.822817	-2.355347
C	-2.226214	0.187070	4.484070
C	-3.427175	0.020817	3.537824
C	-3.350827	0.867343	2.283983
C	-0.882743	-0.329951	3.943345
C	-0.307314	0.442097	2.739512
H	-2.121694	1.248157	4.753734
H	-3.527976	-1.036024	3.253612
H	-0.971646	-1.389412	3.670706
H	0.732622	0.127526	2.582110
H	-2.447509	-0.341760	5.419282
H	-4.352087	0.275813	4.076521
H	-0.141822	-0.273775	4.751472
H	-0.264422	1.517868	2.986295
N	-1.006198	0.230959	1.485946
H	-2.209119	0.513124	1.709869
H	-3.159204	1.926723	2.492497
C	-4.427829	0.654300	1.225589
H	-4.122238	1.147102	0.294850
H	-4.524141	-0.414815	1.003234
C	-5.761741	1.202543	1.677297
C	-6.852106	0.471146	1.912048
H	-5.802992	2.282586	1.825260
H	-7.785015	0.924516	2.234590
H	-6.854805	-0.608008	1.776964

TS3-3a

B3LYP/BS1 SCF energy: -3338.738067 a.u.

M06-L/BS2 SCF energy: -3338.62723 a.u.

M06-L/BS2 Free energy: -3337.849548 a.u.

Fe	-0.205704	0.265743	-0.205991
Cl	-1.692307	1.138838	-1.683798
N	0.277069	-1.731551	-0.393399
N	1.715255	1.025897	-0.243462
C	2.251300	2.276580	-0.276544
C	3.636792	2.215378	0.041284
H	4.313918	3.054167	0.083205
C	3.951230	0.895609	0.273314
C	2.756706	0.143956	0.091740

C	-0.436175	-2.879057	-0.560599
C	1.514170	3.549774	-0.653826
C	0.240960	3.769476	0.210177
H	-0.442272	2.924041	0.102829
C	2.435281	4.785924	-0.448067
H	2.753734	4.842241	0.601025
H	3.342120	4.677590	-1.055410
C	1.112322	3.513133	-2.160158
H	2.018180	3.385370	-2.767258
H	0.466810	2.653304	-2.354526
C	0.386643	4.815667	-2.557229
H	0.104374	4.753285	-3.615821
H	-2.538760	-1.096377	-0.116297
H	-1.634315	-1.424656	-2.575291
C	1.577712	-2.109658	-0.018329
H	4.918511	0.489312	0.530230
C	2.670685	-1.253942	0.198455
C	0.389531	-4.003696	-0.283477
C	-1.874461	-2.966447	-1.039547
H	0.528860	3.819059	1.268995
C	-0.482730	5.067733	-0.205550
C	1.716945	6.090052	-0.848365
C	1.321968	6.020300	-2.337135
C	-0.880891	4.985436	-1.694095
C	-2.841916	-2.145211	-0.142705
C	-1.978755	-2.459395	-2.510032
C	1.636473	-3.529419	0.056464
C	3.956337	-1.944388	0.570245
H	0.089182	-5.038252	-0.342429
C	-2.362062	-4.443331	-1.021468
H	-1.384438	5.182721	0.410475
C	0.452547	6.271785	0.013749
H	2.400373	6.933520	-0.685659
H	2.220203	5.922383	-2.961358
H	0.822294	6.950253	-2.639112
H	-1.561364	4.142234	-1.855936
H	-1.415660	5.898537	-1.988278
H	-2.781861	-2.519923	0.888017
C	-4.289986	-2.249925	-0.665202
C	-3.433067	-2.563042	-3.015131
H	-1.315340	-3.063983	-3.142441
H	2.509593	-4.110802	0.314265
C	4.305629	-2.192319	1.908847
C	4.873310	-2.375260	-0.405735
H	-1.709369	-5.056919	-1.654486
H	-2.294850	-4.845285	-0.002060
C	-3.812568	-4.556445	-1.532579
H	-0.058687	7.205197	-0.256265
H	0.726342	6.352149	1.074502
C	-4.356606	-1.718868	-2.112481
C	-4.744631	-3.721492	-0.633463
H	-4.943380	-1.647386	-0.020920
C	-3.889094	-4.034682	-2.981543
H	-3.477187	-2.183693	-4.043872
C	5.494201	-2.828792	2.265699
C	6.068242	-3.013683	-0.073648
H	-4.115785	-5.611065	-1.502546
H	-4.051732	-0.667014	-2.142882
H	-5.389743	-1.770420	-2.481741
H	-5.782302	-3.806858	-0.982070
H	-4.720868	-4.104450	0.395766
H	-3.252486	-4.644489	-3.636429
H	-4.915950	-4.123830	-3.360084
H	5.718489	-2.996564	3.312676
C	6.373891	-3.237867	1.266489
H	6.743144	-3.327196	-0.861609
H	7.301780	-3.733887	1.533463
Cl	3.228511	-1.694104	3.204354
Cl	4.530519	-2.114968	-2.105768
C	-0.358572	0.216327	2.823694
C	-2.820768	1.754263	2.398047
H	-1.848630	1.212078	1.675037
C	-1.512202	0.143420	3.841694
H	0.364364	0.984493	3.149813
H	0.179897	-0.741419	2.809058
C	-2.324736	1.453444	3.803560

H	-2.156750	-0.708125	3.593745
H	-1.110862	-0.030944	4.846396
H	-3.170554	1.378876	4.502534
H	-1.692565	2.275152	4.160191
N	-0.840678	0.485202	1.488071
C	-4.085708	1.072613	1.914535
H	-4.080229	0.015212	2.203817
H	-4.115169	1.097742	0.818716
H	-2.761285	2.807950	2.109655
C	-5.376945	1.735779	2.461438
H	-5.379628	1.706564	3.557674
H	-5.372797	2.796198	2.171281
C	-6.619379	1.072761	1.932819
C	-7.526351	0.438508	2.676677
H	-6.755826	1.116379	0.851222
H	-8.401510	-0.029791	2.235931
H	-7.429171	0.369130	3.758035

TS4-3a

B3LYP/BS1 SCF energy: -3338.724754 a.u.

M06-L/BS2 SCF energy: -3338.609214 a.u.

M06-L/BS2 Free energy: -3337.831103 a.u.

Fe	-0.065213	0.171878	-0.454954
Cl	-1.258573	0.644941	-2.320229
N	0.762507	-1.714974	-0.338505
N	1.650520	1.265152	-0.153540
C	1.956275	2.592856	-0.181820
C	3.250314	2.798776	0.368431
H	3.751914	3.748848	0.466837
C	3.743491	1.568354	0.742849
C	2.751306	0.603727	0.416859
C	0.291806	-2.978633	-0.517796
C	1.084339	3.693464	-0.760461
C	-0.353995	3.672955	-0.172801
H	-0.833236	2.710201	-0.365922
C	1.696703	5.088007	-0.444673
H	1.784163	5.219251	0.641754
H	2.709991	5.150303	-0.859673
C	1.008329	3.560233	-2.312628
H	2.025294	3.607156	-2.723697
H	0.592704	2.587360	-2.584877
C	0.141595	4.689539	-2.908433
H	0.092805	4.558991	-3.996890
H	-2.110219	-1.553412	-0.691443
H	-0.693246	-1.945321	-2.879337
C	2.013697	-1.829322	0.290973
H	4.704352	1.357581	1.189062
C	2.886471	-0.780334	0.619935
C	1.225904	-3.918439	0.002939
C	-0.994003	-3.356733	-1.232785
H	-0.297071	3.789241	0.918131
C	-1.211339	4.800319	-0.785456
C	0.840292	6.221974	-1.043733
C	0.769433	6.056729	-2.575073
C	-1.281078	4.619421	-2.316254
C	-2.236145	-2.636563	-0.639880
C	-0.877489	-3.014390	-2.750412
C	2.291455	-3.208819	0.506748
C	4.178413	-1.204835	1.266077
H	1.115884	-4.991564	-0.008245
C	-1.243855	-4.887646	-1.120439
H	-2.222795	4.745665	-0.361927
C	-0.581545	6.166254	-0.453103
H	1.306618	7.184387	-0.796231
H	1.775262	6.129153	-3.009892
H	0.172456	6.867009	-3.014214
H	-1.742799	3.656428	-2.561177
H	-1.909427	5.404949	-2.756971
H	-2.329241	-2.895426	0.423412
C	-3.515702	-3.041043	-1.401867
C	-2.166177	-3.419793	-3.495990
H	-0.014327	-3.547628	-3.170057
H	3.183979	-3.607044	0.966755
C	4.311976	-1.304286	2.661689
C	5.317223	-1.522053	0.503807

H	-0.393019	-5.434733	-1.544431
H	-1.318428	-5.175610	-0.063599
C	-2.527664	-5.299612	-1.868833
H	-1.194417	6.978267	-0.865941
H	-0.545329	6.313656	0.634806
C	-3.370692	-2.668407	-2.892084
C	-3.738225	-4.559389	-1.268337
H	-4.369174	-2.501957	-0.969896
C	-2.388701	-4.938322	-3.361499
H	-2.059559	-3.152108	-4.554886
C	5.503190	-1.696230	3.272020
C	6.519523	-1.916153	1.091189
H	-2.665815	-6.383354	-1.761653
H	-3.230372	-1.586894	-2.998365
H	-4.288223	-2.933515	-3.434374
H	-4.658810	-4.856101	-1.788113
H	-3.863899	-4.834235	-0.212300
H	-1.547160	-5.486573	-3.805668
H	-3.291679	-5.240904	-3.908058
H	5.556027	-1.757945	4.352802
C	6.606373	-2.001755	2.478600
H	7.370124	-2.150272	0.461558
H	7.538174	-2.307722	2.943826
Cl	2.948105	-0.927907	3.702834
Cl	5.253935	-1.426380	-1.246125
C	-0.933914	0.425630	2.470899
C	-2.371019	0.392029	3.028337
H	-0.432968	1.363513	2.761888
H	-0.304784	-0.401267	2.822296
C	-3.166584	1.148876	1.962355
H	-2.725324	-0.644050	3.079084
H	-2.456441	0.825919	4.031578
H	-3.031436	2.235049	2.005185
N	-1.108090	0.348535	1.024836
H	-2.306744	0.799774	0.997627
C	-4.568966	0.717950	1.609248
C	-5.591194	1.040033	2.722414
H	-4.581692	-0.362253	1.412635
H	-4.885542	1.213754	0.682643
H	-5.574629	2.118339	2.930265
H	-5.297338	0.540225	3.653399
C	-7.023858	0.610516	2.348916
H	-7.301319	1.105458	1.406493
H	-7.046136	-0.469002	2.154430
C	-8.029759	0.956173	3.412465
C	-8.770194	0.074992	4.085621
H	-8.134025	2.018362	3.640233
H	-9.477493	0.386196	4.848819
H	-8.699646	-0.993372	3.893345