

Supporting Information for

Experimentally Quantifying Small Molecule Bond

Activation Using K β X-ray Emission Spectroscopy

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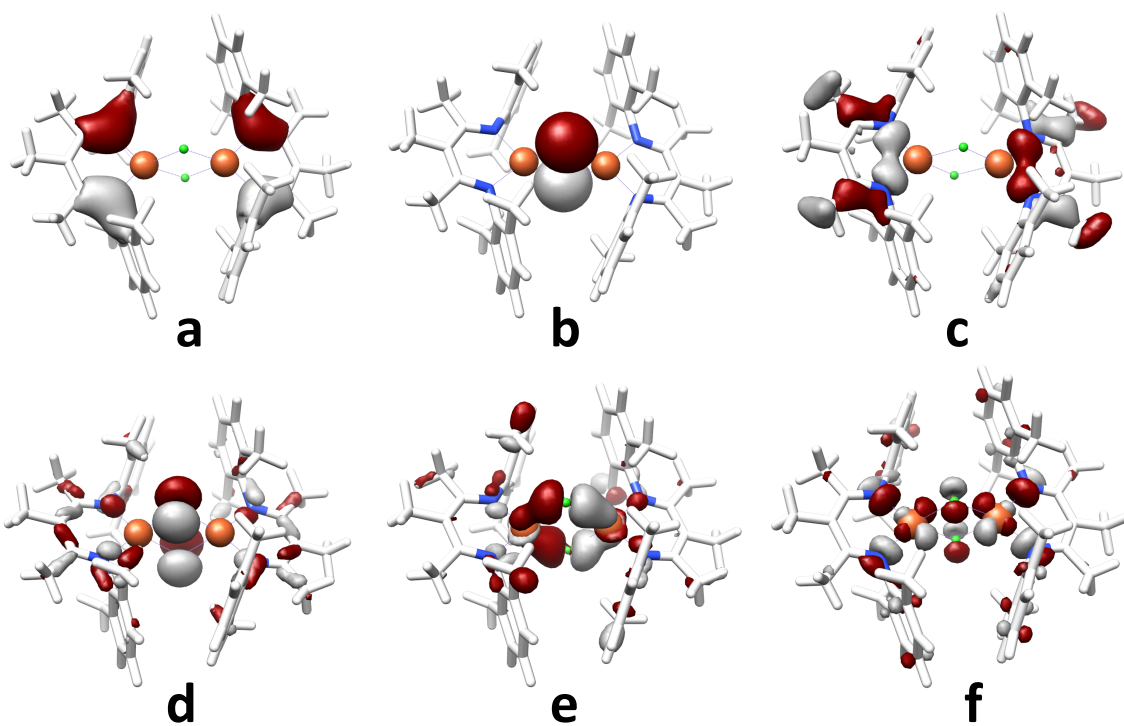
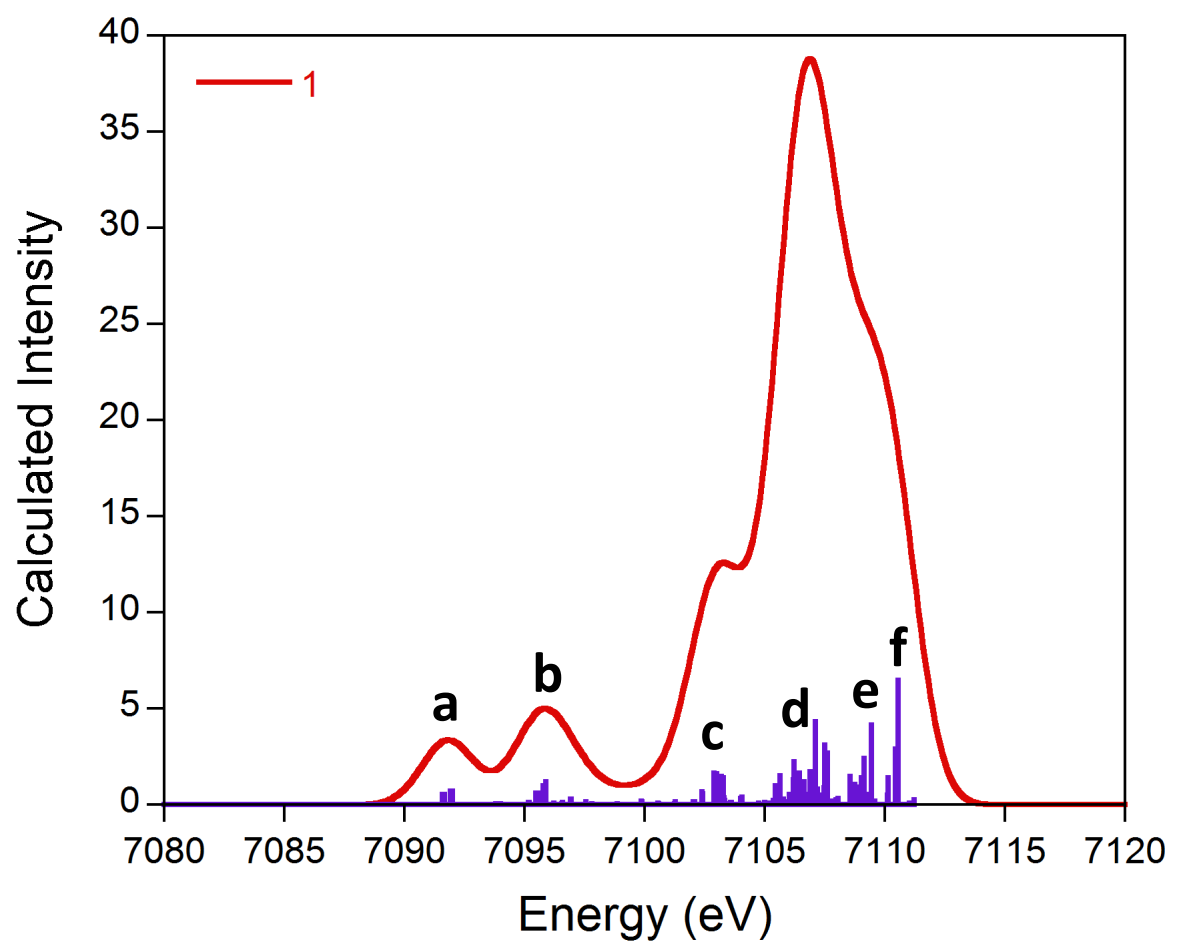
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Figure S1: Assignment of the XES spectrum of **1**.



Sample ORCA Geometry Optimization Input File

```
! UKS BP86 def2-TZVP def2-TZV/J TightSCF SlowConv SCFConv7
! Grid4 NoFinalGrid Normalprint
! PAL6
! MOREAD
! OPT

%moinp"LFeNNFeLK2_opt5_2.gbw"

%maxcore 1024

%plots format cube
    dim1 60 dim2 60 dim3 60
    SpinDens("tBuLFeNNFeLK2_opt5_3.cube");
end

%basis newgto Fe "CP(PPP)" end
    end

%method SpecialGridAtoms 26
    SpecialGridIntAcc 7
    end

* xyzfile 0 5 LFeNNFeLK2_opt5_2.xyz
```

Sample ORCA XES Calculation

```
! UKS BP86 def2-TZVP def2-TZV/J TightSCF SlowConv SCFConv7
! Grid4 NoFinalGrid Normalprint
! PAL6
! MOREAD NOITER

%moinp"LFeNNFeLK2_opt5_3.gbw"

%maxcore 1024

%basis newgto Fe "CP(PPP)" end
    end

%method SpecialGridAtoms 26
    SpecialGridIntAcc 7
    end

%xes CoreOrb 0,0
    OrbOp 0,1
    end

* xyzfile 0 5 LFeNNFeLK2_opt5_3.xyz
```

Optimized Coordinates for 1

Fe	-0.310844	0.695959	-1.564179
Fe	0.310636	-0.696173	1.564223
Cl	0.550963	1.515856	0.500205
N	-1.910330	1.410445	-2.463044
N	0.758752	0.796808	-3.214358
C	-3.432531	1.971057	-4.328520
H	-3.983453	2.523243	-3.559829
H	-4.075403	1.139041	-4.659975
H	-3.286684	2.629716	-5.194684
C	-2.103356	1.459393	-3.797952
C	-1.115434	1.092765	-4.751684
C	0.262109	0.894905	-4.465046
C	1.221795	0.831969	-5.641903
H	2.258361	0.978105	-5.320158
H	0.979631	1.593545	-6.395060
H	1.166874	-0.147661	-6.144272
C	-1.543882	1.022320	-6.209799
H	-2.587495	0.697710	-6.306528
H	-0.942280	0.295422	-6.769695
H	-1.457098	1.987952	-6.741541
C	-2.925296	1.912027	-1.582198
C	-2.857381	3.256652	-1.143089
C	-3.884198	3.748047	-0.325665
H	-3.842959	4.788385	0.006248
C	-4.956794	2.937198	0.049017
H	-5.756568	3.340295	0.673571
C	-5.000133	1.608531	-0.375841
H	-5.831779	0.966841	-0.077424
C	-3.992166	1.069876	-1.186951
C	-1.718287	4.152211	-1.558227
H	-1.881346	5.178058	-1.201429
H	-1.594875	4.181641	-2.651152
H	-0.764151	3.796623	-1.138826
C	-4.065204	-0.365097	-1.643296
H	-4.920611	-0.872906	-1.178767
H	-3.151576	-0.915460	-1.375152
H	-4.176682	-0.442908	-2.736089
C	2.177566	0.757576	-3.010759
C	2.863082	-0.479841	-3.049605
C	4.255790	-0.474359	-2.892415
H	4.791052	-1.425252	-2.930229
C	4.958060	0.714420	-2.689868
H	6.043748	0.697747	-2.575304
C	4.265970	1.925382	-2.631957
H	4.810171	2.859362	-2.471566
C	2.874842	1.970733	-2.792248
C	2.127387	-1.774080	-3.288012
H	2.810557	-2.627929	-3.189675
H	1.681442	-1.810618	-4.294531
H	1.305708	-1.906905	-2.569384
C	2.143648	3.288171	-2.753536
H	2.848155	4.119016	-2.614064
H	1.419142	3.313457	-1.925279
H	1.574954	3.470177	-3.678219

Cl	-0.551368	-1.516002	-0.500089
N	1.910310	-1.410216	2.463119
N	-0.758991	-0.797443	3.214322
C	3.432543	-1.970487	4.328719
H	3.983656	-2.522595	3.560114
H	4.075179	-1.138270	4.660130
H	3.286823	-2.629107	5.194934
C	2.103245	-1.459250	3.798047
C	1.115184	-1.092899	4.751731
C	-0.262405	-0.895413	4.465036
C	-1.222210	-0.832831	5.641812
H	-2.258724	-0.979067	5.319944
H	-0.980005	-1.594520	6.394846
H	-1.167472	0.146704	6.144380
C	1.543585	-1.022414	6.209860
H	2.587147	-0.697648	6.306623
H	0.941861	-0.295620	6.769759
H	1.456928	-1.988072	6.741575
C	2.925605	-1.911163	1.582284
C	2.858337	-3.255700	1.142793
C	3.885469	-3.746391	0.325333
H	3.844731	-4.786650	-0.006891
C	4.957750	-2.934959	-0.048983
H	5.757793	-3.337532	-0.673531
C	5.000443	-1.606387	0.376241
H	5.831843	-0.964247	0.078100
C	3.992140	-1.068416	1.187381
C	1.719603	-4.151902	1.557517
H	1.883381	-5.177656	1.200776
H	1.595812	-4.181397	2.650394
H	0.765421	-3.796870	1.137749
C	4.064405	0.366484	1.644074
H	4.919637	0.874821	1.179796
H	3.150539	0.916447	1.375914
H	4.175678	0.444103	2.736903
C	-2.177798	-0.758545	3.010607
C	-2.863475	0.478810	3.048662
C	-4.256203	0.473039	2.891684
H	-4.791579	1.423902	2.928827
C	-4.958344	-0.715982	2.690123
H	-6.044057	-0.699541	2.575758
C	-4.266102	-1.926886	2.632904
H	-4.810217	-2.861051	2.473295
C	-2.874938	-1.971945	2.792965
C	-2.127876	1.773323	3.285850
H	-2.811103	2.627041	3.186716
H	-1.681925	1.810832	4.292335
H	-1.306221	1.905514	2.567076
C	-2.143605	-3.289323	2.755134
H	-2.848039	-4.120343	2.616333
H	-1.419179	-3.315137	1.926833
H	-1.574817	-3.470590	3.679905

Optimized Coordinates for 2

Fe	0.002105	0.095227	2.383217
Fe	-0.041056	-0.049619	-2.402487
N	0.001803	0.037533	0.580547
N	-1.460677	0.093969	3.705089
N	1.481401	0.101572	3.687068
C	-2.416406	0.102088	6.131278
C	-1.277000	0.123194	5.041694
C	0.023370	0.120901	5.593286
H	0.030481	0.123972	6.676792
C	1.316494	0.104078	5.025332
C	2.470468	0.175026	6.095998
C	-2.258008	-1.191523	6.972900
H	-2.365819	-2.086058	6.342019
H	-3.039638	-1.226791	7.748381
H	-1.282544	-1.251358	7.473009
C	-3.874520	0.119749	5.629619
H	-4.121705	1.031034	5.073309
H	-4.531905	0.081903	6.512760
H	-4.122989	-0.737925	4.995218
C	-2.271696	1.338106	7.058700
H	-2.360328	2.272540	6.484878
H	-1.315582	1.364206	7.596391
H	-3.076986	1.327051	7.810014
C	3.920761	0.155353	5.571640
H	4.169929	-0.774330	5.047261
H	4.592063	0.235194	6.441344
H	4.148549	0.990107	4.899954
C	2.352932	-1.029482	7.066695
H	2.438764	-1.982755	6.524362
H	1.406953	-1.044406	7.622781
H	3.170724	-0.985535	7.803062
C	2.303578	1.492351	6.898822
H	1.332985	1.552750	7.408393
H	2.390654	2.368313	6.239434
H	3.093842	1.563097	7.663033
C	-2.714454	0.134775	3.013462
C	-3.289703	1.393406	2.685524
C	-4.463795	1.411531	1.923289
H	-4.923604	2.369271	1.671887
C	-5.072060	0.229512	1.496324
H	-5.992035	0.266967	0.909643
C	-4.505160	-0.998588	1.835849
H	-4.992003	-1.921468	1.511705
C	-3.328708	-1.075557	2.593672
C	-2.651201	2.697005	3.158799
H	-1.997185	2.448469	4.008346
C	-3.674948	3.736038	3.651052
H	-3.153708	4.601437	4.087713
H	-4.343943	3.320224	4.418830
H	-4.302294	4.115155	2.829988
C	-1.756045	3.306066	2.063870
H	-1.232296	4.199201	2.437226
H	-2.350303	3.598938	1.186244
H	-0.999284	2.585028	1.717598

C	-2.750527	-2.440237	2.953665
H	-1.886578	-2.266325	3.612723
C	-3.757421	-3.321042	3.719587
H	-4.130291	-2.827609	4.628692
H	-3.282504	-4.268163	4.018709
H	-4.628779	-3.572088	3.095434
C	-2.251033	-3.182343	1.700654
H	-1.531372	-2.578985	1.130618
H	-3.089258	-3.423100	1.029319
H	-1.761939	-4.128777	1.976700
C	2.721291	0.023751	2.975478
C	3.330337	1.212650	2.495106
C	4.488161	1.099831	1.712948
H	4.974305	2.007163	1.346772
C	5.042549	-0.143081	1.411018
H	5.948494	-0.208623	0.805319
C	4.443887	-1.304436	1.905374
H	4.893856	-2.272935	1.679850
C	3.287536	-1.250714	2.691698
C	2.778577	2.594251	2.832638
H	1.914791	2.446888	3.498686
C	2.282423	3.324545	1.571978
H	1.540588	2.728680	1.022896
H	3.116707	3.531662	0.884639
H	1.821038	4.288108	1.836157
C	3.804844	3.467912	3.581684
H	4.167753	2.982874	4.499231
H	3.351792	4.430919	3.863717
H	4.680782	3.686324	2.951726
C	2.648728	-2.529021	3.230456
H	2.071484	-2.250031	4.125255
C	1.650418	-3.120982	2.218765
H	0.894945	-2.377374	1.919411
H	1.125414	-3.988519	2.646464
H	2.163075	-3.446311	1.302007
C	3.670985	-3.596995	3.657146
H	4.413410	-3.195541	4.362610
H	4.215881	-4.012323	2.795737
H	3.154878	-4.435991	4.148022
N	-0.000632	0.006856	-0.599184
N	-0.100274	1.366981	-3.772068
N	0.039355	-1.567467	-3.655393
C	-0.097407	2.241320	-6.227420
C	-0.083688	1.139406	-5.101603
C	-0.042866	-0.177660	-5.610169
H	-0.027838	-0.219835	-6.692976
C	0.017271	-1.449275	-4.998529
C	0.046691	-2.639926	-6.029803
C	0.000217	3.712843	-5.776357
H	-0.819082	4.017927	-5.117409
H	-0.045845	4.343084	-6.678667
H	0.942796	3.938273	-5.264242
C	-1.423000	2.108424	-7.022838
H	-2.291694	2.271465	-6.368184
H	-1.537045	1.121373	-7.489405
H	-1.452896	2.866948	-7.821148

C	1.098549	2.007295	-7.187599
H	1.098964	2.785035	-7.967436
H	1.061814	1.032469	-7.690712
H	2.054945	2.071224	-6.647778
C	-1.151954	-2.507301	-7.005659
H	-1.141053	-3.351291	-7.713089
H	-1.128251	-1.581500	-7.594647
H	-2.108214	-2.536046	-6.462416
C	1.371293	-2.555309	-6.833494
H	2.241669	-2.657318	-6.168900
H	1.472842	-1.605209	-7.373984
H	1.410323	-3.372769	-7.570992
C	-0.038515	-4.068589	-5.454762
H	0.784453	-4.310439	-4.774426
H	0.010732	-4.773144	-6.300127
H	-0.979317	-4.256407	-4.923557
C	-0.063232	2.641816	-3.120807
C	1.194076	3.251238	-2.853495
C	1.213884	4.447572	-2.127281
H	2.169693	4.933760	-1.922663
C	0.034629	5.043619	-1.675138
H	0.072898	5.981281	-1.117239
C	-1.191695	4.440122	-1.951091
H	-2.112723	4.915712	-1.605764
C	-1.270696	3.240186	-2.671242
C	2.494676	2.621758	-3.347198
H	2.233416	1.938923	-4.169727
C	3.150208	1.770318	-2.243452
H	2.454246	1.009087	-1.857793
H	3.451827	2.395877	-1.390544
H	4.044906	1.254838	-2.624541
C	3.499760	3.648310	-3.899452
H	3.051810	4.283690	-4.677629
H	4.363952	3.129024	-4.341008
H	3.888061	4.308771	-3.109291
C	-2.636517	2.619021	-2.953964
H	-2.468701	1.732911	-3.584979
C	-3.575420	3.573679	-3.719384
H	-3.136097	3.915249	-4.667161
H	-3.812125	4.467040	-3.121217
H	-4.526419	3.068859	-3.949551
C	-3.316595	2.149777	-1.655586
H	-2.676555	1.461866	-1.086542
H	-4.263373	1.633900	-1.876108
H	-3.547799	3.005387	-1.003158
C	0.049102	-2.781866	-2.897495
C	1.276086	-3.295787	-2.401406
C	1.239775	-4.426953	-1.574192
H	2.176964	-4.836696	-1.190122
C	0.035525	-5.043787	-1.239277
H	0.029780	-5.925131	-0.595011
C	-1.164625	-4.533547	-1.740065
H	-2.102031	-5.031045	-1.485375
C	-1.187329	-3.407587	-2.570684
C	2.617035	-2.656377	-2.752725
H	2.414855	-1.853318	-3.477741

C	3.275249	-2.015567	-1.517916
H	2.607639	-1.290215	-1.033001
H	4.203171	-1.493961	-1.797529
H	3.535071	-2.780264	-0.770247
C	3.592119	-3.653434	-3.411181
H	3.162843	-4.119155	-4.309625
H	3.868799	-4.461894	-2.717122
H	4.520121	-3.139772	-3.706454
C	-2.505014	-2.860501	-3.113824
H	-2.275787	-2.347899	-4.060918
C	-3.543690	-3.952155	-3.421841
H	-3.132163	-4.736413	-4.074250
H	-4.414047	-3.509319	-3.929171
H	-3.915540	-4.436787	-2.506122
C	-3.106832	-1.805912	-2.167182
H	-4.005791	-1.349406	-2.608404
H	-2.386545	-0.998939	-1.953349
H	-3.384669	-2.251789	-1.201299

Optimized Coordinates for 3

Fe	0.010515	-0.009509	2.378698
Fe	0.125817	0.007114	-2.386886
K	0.944994	2.559754	0.035420
K	-0.793182	-2.576612	-0.025309
N	0.055061	-0.007249	0.610672
N	0.085983	-0.003262	-0.618378
N	-0.099794	1.453137	3.711084
N	0.056861	-1.475158	3.712556
N	1.056641	1.172193	-3.693997
N	-0.748266	-1.139827	-3.747568
C	-0.374218	2.397058	6.143623
C	-0.152846	1.275620	5.054576
C	-0.071309	-0.012964	5.613918
H	-0.098701	-0.013765	6.696861
C	0.041528	-1.300419	5.057316
C	0.215838	-2.422725	6.154091
C	-1.735304	2.120590	6.834693
H	-2.560474	2.184225	6.110262
H	-1.915931	2.871211	7.620676
H	-1.774709	1.126392	7.297134
C	-0.425603	3.864689	5.675479
H	-1.213985	4.052696	4.939788
H	0.521799	4.214970	5.250260
H	-0.642565	4.489234	6.556226
C	0.753139	2.336104	7.205702
H	1.737645	2.505629	6.746260
H	0.793517	1.377778	7.738070
H	0.592632	3.125124	7.957108
C	0.282132	-3.890567	5.688339
H	1.098943	-4.082149	4.985488
H	-0.648497	-4.237311	5.224812
H	0.460167	-4.515664	6.577383
C	-0.952671	-2.360830	7.170803
H	-1.010696	-1.404624	7.705321
H	-0.824569	-3.153075	7.924987
H	-1.919001	-2.525081	6.672468
C	1.548167	-2.147442	6.899333
H	1.568778	-1.152867	7.362304
H	2.401926	-2.211554	6.208907
H	1.696513	-2.897802	7.692319
C	0.068501	2.716302	3.087787
C	1.366709	3.316678	3.031193
C	1.518983	4.544947	2.373223
H	2.504627	5.013292	2.340288
C	0.436512	5.194329	1.770724
H	0.574974	6.157567	1.277585
C	-0.828143	4.601549	1.828228
H	-1.679339	5.116120	1.376378
C	-1.041725	3.381417	2.484596
C	2.582415	2.627097	3.646572
H	2.207452	1.914428	4.394784
C	3.540235	3.594622	4.359631
H	3.016475	4.218015	5.098671
H	4.050338	4.268063	3.654098

H	4.322269	3.028101	4.886532
C	3.335908	1.802205	2.585767
H	2.669815	1.044285	2.138971
H	4.189655	1.272499	3.034589
H	3.731000	2.451989	1.787212
C	-2.452227	2.806677	2.561237
H	-2.401249	1.930177	3.224032
C	-3.471837	3.798908	3.150330
H	-3.175825	4.156587	4.146362
H	-4.455227	3.314355	3.245502
H	-3.602662	4.680266	2.504130
C	-2.926517	2.315672	1.183635
H	-2.238468	1.556832	0.784532
H	-2.990472	3.147153	0.464434
H	-3.926105	1.861437	1.256772
C	-0.068760	-2.737366	3.077777
C	1.076145	-3.389052	2.527272
C	0.906605	-4.608275	1.856574
H	1.783988	-5.113250	1.445712
C	-0.348189	-5.211723	1.732907
H	-0.452910	-6.173907	1.229434
C	-1.465315	-4.575427	2.284147
H	-2.443619	-5.052779	2.200798
C	-1.356943	-3.349279	2.954759
C	2.476282	-2.803167	2.676424
H	2.382673	-1.920552	3.326328
C	3.024817	-2.322924	1.322881
H	2.356464	-1.572325	0.877612
H	3.134143	-3.160770	0.616625
H	4.016146	-1.862009	1.447867
C	3.467095	-3.783103	3.332238
H	3.117820	-4.132471	4.313771
H	4.440968	-3.291653	3.477167
H	3.638309	-4.670160	2.703484
C	-2.606602	-2.674197	3.515899
H	-2.274411	-1.970825	4.292670
C	-3.307103	-1.836896	2.428868
H	-2.619558	-1.074387	2.023968
H	-4.182302	-1.312175	2.840694
H	-3.661699	-2.478032	1.604718
C	-3.596416	-3.654509	4.164565
H	-3.109708	-4.286998	4.921024
H	-4.067353	-4.319049	3.424202
H	-4.406485	-3.097488	4.658158
C	1.822630	1.839732	-6.114810
C	0.997665	1.027011	-5.041040
C	0.193224	0.029543	-5.622075
H	0.215782	0.037160	-6.704736
C	-0.633256	-0.976499	-5.088868
C	-1.408615	-1.777844	-6.206912
C	2.692429	3.016020	-5.628965
H	2.106262	3.832738	-5.192678
H	3.223332	3.422653	-6.503979
H	3.449582	2.718563	-4.896876
C	0.866246	2.441588	-7.176374
H	0.143123	3.127721	-6.712376

H	0.298941	1.682073	-7.728342
H	1.450451	3.015762	-7.912502
C	2.790488	0.847523	-6.811091
H	3.370824	1.371082	-7.587639
H	2.260250	0.012371	-7.285764
H	3.500789	0.422612	-6.086761
C	-2.350862	-0.780525	-6.930633
H	-1.805219	0.064072	-7.369820
H	-3.094306	-0.369678	-6.231877
H	-2.894052	-1.295597	-7.739053
C	-0.404943	-2.361677	-7.234449
H	0.180377	-1.592335	-7.752926
H	-0.954100	-2.930110	-8.001350
H	0.302323	-3.049312	-6.748677
C	-2.292665	-2.963842	-5.773440
H	-1.722040	-3.782975	-5.321276
H	-2.782533	-3.362544	-6.675593
H	-3.082829	-2.678354	-5.072004
C	1.667534	2.276042	-3.045404
C	2.965108	2.147174	-2.463193
C	3.518243	3.243602	-1.786812
H	4.516590	3.149545	-1.353036
C	2.842588	4.463110	-1.686099
H	3.303318	5.311276	-1.177660
C	1.574725	4.586508	-2.263569
H	1.050814	5.542038	-2.196153
C	0.968182	3.520568	-2.942549
C	3.770740	0.857538	-2.582505
H	3.196042	0.183400	-3.234698
C	3.918495	0.165067	-1.217525
H	2.933233	-0.065978	-0.788448
H	4.473217	0.797910	-0.507136
H	4.471191	-0.780756	-1.321079
C	5.157484	1.077721	-3.215580
H	5.672174	0.112885	-3.338551
H	5.796793	1.711809	-2.582491
H	5.092436	1.552093	-4.204501
C	-0.427100	3.695488	-3.538303
H	-0.562569	2.900217	-4.284925
C	-0.623210	5.045017	-4.248311
H	-1.595744	5.060905	-4.762258
H	0.159330	5.230882	-4.997943
H	-0.617765	5.889172	-3.542083
C	-1.511906	3.488986	-2.464030
H	-1.432303	2.483235	-2.018447
H	-2.517542	3.580553	-2.901565
H	-1.426382	4.244508	-1.665657
C	-1.384094	-2.251993	-3.138236
C	-0.686579	-3.495961	-3.017535
C	-1.319047	-4.569869	-2.375904
H	-0.796064	-5.524932	-2.295502
C	-2.610723	-4.454921	-1.851588
H	-3.090445	-5.309147	-1.371654
C	-3.285038	-3.236247	-1.970334
H	-4.301387	-3.148613	-1.579180
C	-2.706358	-2.132390	-2.612422

C	0.733552	-3.660931	-3.554537
H	0.897161	-2.859029	-4.288348
C	1.770763	-3.458408	-2.433434
H	1.664031	-2.458273	-1.980607
H	2.794602	-3.537183	-2.829242
H	1.658210	-4.223704	-1.647823
C	0.965323	-5.003623	-4.266510
H	0.216674	-5.185532	-5.050955
H	0.932375	-5.853783	-3.568266
H	1.959320	-5.011909	-4.737811
C	-3.509855	-0.844099	-2.756512
H	-2.914346	-0.167236	-3.386848
C	-4.873486	-1.064930	-3.437348
H	-4.773851	-1.541689	-4.422318
H	-5.382821	-0.100050	-3.580525
H	-5.535345	-1.696950	-2.825791
C	-3.704147	-0.155690	-1.395460
H	-2.733583	0.077947	-0.935497
H	-4.277842	-0.793218	-0.704435
H	-4.257643	0.787939	-1.513906

Optimized Coordinates for 4

Fe	1.999357	0.422090	-0.072343
Fe	0.755905	0.116528	-2.510447
Fe	3.598360	-2.116259	-1.992006
Fe	-3.334497	5.184343	0.619806
N	0.484647	1.189281	-0.954612
N	2.325037	-0.767672	-1.643799
N	3.522716	1.603782	0.785051
N	1.610688	-0.201968	1.894544
C	5.509599	1.942888	2.226882
H	5.525154	2.947355	1.791213
H	6.419653	1.421887	1.887867
H	5.582805	2.032069	3.318775
C	4.259184	1.173427	1.821681
C	3.921280	0.051406	2.633350
C	2.608411	-0.473229	2.755759
C	2.325743	-1.356533	3.959996
H	1.254848	-1.557993	4.068047
H	2.694813	-0.906975	4.893008
H	2.839436	-2.323189	3.838049
C	4.972257	-0.446302	3.611682
H	4.832681	-1.510779	3.832816
H	4.961218	0.089544	4.579744
H	5.986269	-0.345260	3.203346
C	3.880824	2.843056	0.169733
C	3.255249	4.042199	0.593815
C	3.639023	5.255369	0.001471
H	3.166504	6.181306	0.340085
C	4.634881	5.295974	-0.977387
H	4.937673	6.249613	-1.414327
C	5.245538	4.108778	-1.384878
H	6.031664	4.133167	-2.144090
C	4.876376	2.872164	-0.835076
C	2.259359	4.028400	1.724332
H	1.743872	4.993812	1.820026
H	2.757552	3.824019	2.686076
H	1.505011	3.238491	1.601268
C	5.565831	1.605401	-1.264329
H	4.843071	0.787107	-1.412160
H	6.284471	1.263731	-0.501757
H	6.117676	1.755514	-2.201182
C	0.263839	-0.401111	2.309261
C	-0.466860	-1.499323	1.787280
C	-1.812574	-1.657774	2.145877
H	-2.368356	-2.505945	1.741345
C	-2.439800	-0.757812	3.014616
H	-3.489193	-0.891735	3.282989
C	-1.706478	0.303539	3.548931
H	-2.182468	1.003200	4.239977
C	-0.353146	0.495657	3.221069
C	0.229304	-2.515550	0.930153
H	-0.466715	-3.305359	0.623648
H	1.065815	-2.974095	1.479403
H	0.671763	-2.063897	0.025894
C	0.411376	1.615167	3.880671

H	-0.196203	2.530070	3.925020
H	1.340360	1.838273	3.345664
H	0.682817	1.342081	4.914291
N	-0.818333	-1.000632	-3.393686
N	0.667322	1.260765	-4.288263
C	-1.945986	-2.220041	-5.234709
H	-2.714250	-2.435423	-4.484811
H	-1.477765	-3.178523	-5.511374
H	-2.435848	-1.834031	-6.138381
C	-0.910498	-1.232657	-4.711561
C	-0.133376	-0.559752	-5.700286
C	0.475477	0.704338	-5.498813
C	0.887773	1.477722	-6.743105
H	1.206642	2.495811	-6.497719
H	0.073417	1.532227	-7.480150
H	1.732463	0.973370	-7.238415
C	-0.170151	-1.116185	-7.114769
H	0.742536	-0.865972	-7.670162
H	-1.017615	-0.736912	-7.716189
H	-0.241718	-2.211645	-7.118063
C	-1.762021	-1.637626	-2.530272
C	-2.929334	-0.940834	-2.131866
C	-3.858998	-1.589545	-1.304560
H	-4.767738	-1.057139	-1.010888
C	-3.655376	-2.906881	-0.886719
H	-4.396206	-3.405093	-0.258323
C	-2.503483	-3.584959	-1.289746
H	-2.343779	-4.620186	-0.976990
C	-1.541262	-2.968200	-2.102798
C	-3.209569	0.442238	-2.659761
H	-2.328336	1.096297	-2.588259
H	-4.048686	0.916739	-2.131776
H	-3.475933	0.411061	-3.728718
C	-0.319651	-3.721461	-2.556127
H	-0.241170	-4.684375	-2.035100
H	0.597747	-3.136490	-2.375703
H	-0.348249	-3.930324	-3.636821
C	0.844726	2.671710	-4.210592
C	2.131249	3.194715	-3.923352
C	2.291671	4.581758	-3.799036
H	3.284410	4.978308	-3.578609
C	1.209017	5.453030	-3.964249
H	1.350434	6.530982	-3.865374
C	-0.049089	4.933115	-4.275685
H	-0.897972	5.605193	-4.422396
C	-0.252921	3.549144	-4.415675
C	3.306806	2.266663	-3.835474
H	4.229257	2.822479	-3.633893
H	3.440799	1.710611	-4.774661
H	3.174515	1.504911	-3.049579
C	-1.614244	3.045651	-4.824802
H	-2.407360	3.599686	-4.303263
H	-1.732128	1.978981	-4.607478
H	-1.768033	3.180901	-5.908734
N	4.898621	-2.428719	-3.573929
N	4.297174	-3.872099	-1.132442

C	6.041186	-3.801066	-5.293617
H	6.514770	-2.859605	-5.589943
H	5.371277	-4.101899	-6.115940
H	6.816221	-4.573537	-5.212843
C	5.271628	-3.654083	-3.986954
C	5.043511	-4.850331	-3.256512
C	4.761170	-4.905669	-1.864839
C	5.098382	-6.223945	-1.177506
H	5.240506	-6.094303	-0.100043
H	6.011972	-6.661227	-1.599918
H	4.295743	-6.966032	-1.316420
C	5.301278	-6.168836	-3.972134
H	4.686623	-6.976127	-3.553059
H	6.352512	-6.510995	-3.926749
H	5.035002	-6.101716	-5.035058
C	5.335006	-1.306184	-4.349849
C	6.544234	-0.651142	-4.018544
C	6.978130	0.414429	-4.821274
H	7.916884	0.915913	-4.571830
C	6.246438	0.820698	-5.938372
H	6.603406	1.643313	-6.560861
C	5.056184	0.163265	-6.256533
H	4.485021	0.468660	-7.137057
C	4.578710	-0.895830	-5.471900
C	3.303975	-1.608634	-5.833741
H	3.466663	-2.682986	-6.006069
H	2.869386	-1.184046	-6.747938
H	2.558351	-1.528840	-5.027498
C	7.380751	-1.127039	-2.859711
H	8.224648	-0.447256	-2.679359
H	7.789426	-2.133694	-3.044186
H	6.783731	-1.200524	-1.939765
C	4.208502	-4.066452	0.286473
C	3.110954	-4.765367	0.845130
C	3.099412	-5.020874	2.224139
H	2.256227	-5.569006	2.652184
C	4.154938	-4.615831	3.042598
H	4.145692	-4.848970	4.109217
C	5.225322	-3.913838	2.483854
H	6.059888	-3.599480	3.115107
C	5.263961	-3.614907	1.114955
C	2.000488	-5.286953	-0.028162
H	1.127405	-5.565096	0.577244
H	2.312673	-6.181889	-0.589825
H	1.692402	-4.538441	-0.769060
C	6.434031	-2.868304	0.531365
H	7.177036	-2.637549	1.306867
H	6.100669	-1.922272	0.075982
H	6.930759	-3.441281	-0.265969
K	0.281707	3.983520	-1.108824
K	-1.992760	1.243088	0.365553
Cl	-1.556457	4.129495	1.751885
Cl	-2.994530	4.063340	-1.421807
N	-3.331536	7.153771	0.704622
N	-5.156761	5.095472	1.368160
C	-4.113770	9.465995	1.039437

H	-3.054368	9.701289	0.888634
H	-4.444414	9.939406	1.974641
H	-4.678528	9.942932	0.221931
C	-4.346491	7.964067	1.066243
C	-5.624910	7.490672	1.471393
C	-5.974444	6.125745	1.664924
C	-7.342744	5.814297	2.249667
H	-7.420188	4.760894	2.540972
H	-8.145694	6.015905	1.522006
H	-7.549384	6.434398	3.133167
C	-6.689086	8.533355	1.782704
H	-6.569074	9.434330	1.168652
H	-6.678759	8.863353	2.838263
H	-7.699680	8.158782	1.578156
C	-2.050969	7.671117	0.341177
C	-1.763116	7.923318	-1.024344
C	-0.476155	8.362523	-1.368009
H	-0.253892	8.572360	-2.417244
C	0.506615	8.558157	-0.394637
H	1.500264	8.908632	-0.680901
C	0.203917	8.324258	0.949017
H	0.962007	8.496693	1.717191
C	-1.068661	7.886116	1.341570
C	-2.823307	7.753992	-2.082418
H	-2.441910	8.064912	-3.064725
H	-3.717120	8.355688	-1.858059
H	-3.153727	6.706034	-2.152195
C	-1.389404	7.663965	2.796488
H	-0.514087	7.879851	3.423991
H	-1.695605	6.622322	2.973539
H	-2.217435	8.307380	3.132531
C	-5.556624	3.740835	1.578199
C	-5.252075	3.102690	2.807889
C	-5.599832	1.753717	2.968147
H	-5.380093	1.262438	3.919270
C	-6.236210	1.043624	1.947237
H	-6.506093	-0.004296	2.092823
C	-6.545926	1.688589	0.747255
H	-7.068085	1.145595	-0.044720
C	-6.224280	3.038296	0.542230
C	-4.590495	3.863330	3.927795
H	-4.504044	3.235118	4.824888
H	-5.159413	4.766511	4.196277
H	-3.581867	4.194442	3.635999
C	-6.604775	3.729268	-0.741816
H	-7.279698	4.579486	-0.558248
H	-7.115521	3.031676	-1.419567
H	-5.716594	4.126406	-1.255508