

Supporting Information: Multireference Protonation Energetics of a Dimeric Model of Nitrogenase Iron–Sulfur Clusters

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I. CLUSTER GEOMETRIES

Cluster geometries are given in XYZ coordinates with the unit Angstrom.

A. Optimized with def2-SV(P)/UKS-TPSS/DFTD3

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27
HC, Energy = -4717.139080700 H
C    -1.0654597    -1.6165964    -3.6938910
H    -1.4383635    -0.5689779    -3.6741341
H    -1.7807115    -2.2443224    -3.1121367
H    -1.0773907    -1.9924332    -4.7494055
S     0.6243829    -1.6537410    -2.9602556
C     0.4156598     1.7876147    -4.0556776
H     1.3488982     2.3835358    -3.9218054
H    -0.1330190     2.2251636    -4.9293434
H     0.7135941     0.7422418    -4.2919146
S    -0.6070437     1.7896179    -2.5222937
C    -0.8232495     2.8573739     1.4681234
H    -0.0877151     2.8066116     0.6407689
H    -0.9439809     3.9246222     1.7897946
H    -1.7975667     2.5226444     1.0498580
S    -0.2735647     1.7807874     2.8579066
C    -1.0643237    -1.5242334     4.0337374
H    -1.0304628    -1.8368555     5.1103107
H    -1.8734238    -2.1231958     3.5494502
H    -1.3541746    -0.4526895     3.9781077
S     0.5588840    -1.7538671     3.1864833
Fe     0.4943827     0.0464709    -1.2052434
Fe     0.5810012    -0.0475200     1.4684925
S     2.2702018     0.5987571     0.0818694
C    -0.9804810    -0.8504359     0.1595883
H    -0.9278775    -1.9603768     0.2106940
H    -1.5301625    -0.5677658    -0.7796813
H    -1.6330329    -0.4914309     0.9945982
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Listing S1. HC

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27
HS, Energy = -4717.096074143 H
C    -1.4481492    -1.2918793    -4.0685921
H    -1.5592125    -0.1859823    -4.0893224
H    -2.3309980    -1.7079134    -3.5297987
H    -1.4760151    -1.6885040    -5.1175674
S     0.1243831    -1.7171690    -3.2045707
C     1.0341701     1.7983129    -3.6269368
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H	1.9627435	1.9656559	-3.0387507
H	0.9926332	2.5651117	-4.4445661
H	1.1042400	0.7824705	-4.0723829
S	-0.4446417	1.8649325	-2.5294114
C	-1.1427404	2.6271747	1.3777265
H	-0.7051544	2.6282955	0.3581567
H	-1.2853067	3.6896251	1.7066593
H	-2.1508112	2.1651199	1.2944240
S	-0.0778785	1.6928495	2.5587062
C	-0.7929520	-1.4324890	4.2467679
H	-0.9625390	-0.3357608	4.1885620
H	-0.5400427	-1.7119510	5.3045419
H	-1.7588854	-1.9373028	4.0010839
S	0.5386887	-1.8989304	3.0569739
Fe	-0.0624496	-0.2245743	-1.3014183
Fe	0.1805793	-0.3587873	1.2612831
S	2.1356417	0.1952062	-0.2457191
C	-1.2915962	-0.9617811	0.0689167
H	1.9086364	1.5088483	0.0713138
H	-2.2983991	-0.4932717	0.2239739
H	-1.4219432	-2.0743068	0.0479475

Listing S2. HS

27
HFe, Energy = -4717.084045403 H

C	-1.7030912	-0.2687576	-3.8857510
H	-1.4276567	0.6161659	-3.2739484
H	-2.7282115	-0.5817080	-3.5791673
H	-1.7544034	0.0472283	-4.9585791
S	-0.4654014	-1.5971491	-3.6068456
C	1.3427752	1.2911521	-3.6530591
H	2.4027725	1.5361646	-3.9146487
H	0.7051324	2.0932763	-4.0999022
H	1.0611069	0.3183708	-4.1168671
S	1.1257526	1.1531598	-1.8302475
C	-0.5460690	2.6148722	1.2254132
H	0.3817785	2.2964072	1.7410684
H	-0.7581861	3.6865849	1.4682270
H	-0.3516724	2.5166490	0.1383690
S	-1.9524226	1.5437145	1.7437219
C	-1.2593992	-1.2001762	4.2059136
H	-0.1794134	-1.4477025	4.1290192
H	-1.6496014	-1.5773749	5.1869269
H	-1.3493637	-0.0933792	4.1760396
S	-2.1872294	-1.9182902	2.7849438
Fe	0.2293122	-1.0722584	-1.1389980
Fe	-1.0895429	-0.6236298	1.1100321
S	1.1201274	-0.6801252	1.0718109
C	-1.6833719	-1.3940353	-0.5791815
H	1.1279016	-2.5680078	-1.3656985
H	-2.5031122	-0.8682227	-1.1171969
H	-1.7445096	-2.4939284	-0.7433938

Listing S3. HFe

27
HFe2, Energy = -4717.102540727 H

C	-0.6004690	-1.8541396	-4.3931123
H	-0.9885128	-0.8116508	-4.4441158
H	-1.2233186	-2.5109691	-5.0545639
H	0.4332653	-1.8614472	-4.8208224
S	-0.6420813	-2.4169491	-2.6407698
C	0.4911160	1.7119732	-3.4952934
H	1.1454118	1.7908560	-2.6017265
H	0.4940557	2.6834804	-4.0526033
H	0.9297739	0.9375322	-4.1667404
S	-1.2045031	1.2624527	-2.9490191
C	-0.5170233	2.7735147	1.7890395
H	0.1897341	2.5579946	0.9587402
H	-0.1817476	3.6864329	2.3434608

H	-1.5092436	2.9968065	1.3360800
S	-0.5859628	1.3069271	2.8986914
C	-0.5055631	-1.6440394	4.3765240
H	-1.3125977	-0.8903412	4.5041769
H	0.4429013	-1.1359999	4.6628636
H	-0.6817372	-2.4716890	5.1124802
S	-0.4582362	-2.2773941	2.6480953
Fe	-0.5822491	-0.4261876	-1.2438221
Fe	-0.4040092	-0.3452652	1.1749566
S	1.3672017	0.2724370	-0.2315191
C	-2.0078868	0.0019752	0.0519971
H	-0.5166457	-1.6358452	-0.0228939
H	-2.3493298	1.0582445	-0.0027923
H	-2.8433420	-0.7077099	0.2366894

Listing S4. HFe₂**B. Optimized with def2-TZVP/UKS-TPSS/DFTD3**

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27
HC, Energy = -5076.012745 H
C -1.89342031 -2.94949331 -7.12177899
H -2.54339731 -0.97906391 -7.09286332
H -3.30953872 -4.10746983 -6.13271285
H -1.78233191 -3.61259806 -9.09765127
S 1.20164028 -3.14391237 -5.53655396
C 0.70175561 3.31623544 -7.75340011
H 2.42278875 4.48645307 -7.75437981
H -0.55001429 4.01726270 -9.26916545
H 1.25567282 1.35936496 -8.16726945
S -0.88385618 3.42838856 -4.65419662
C -1.59341328 5.38738577 2.69823716
H -0.16329228 5.34717827 1.20448660
H -1.86184135 7.35300309 3.34781319
H -3.37275285 4.72943706 1.86139269
S -0.60598410 3.33049089 5.32345806
C -1.97412845 -2.92554715 7.85809788
H -1.77207663 -3.52650830 9.84758262
H -3.52264699 -4.03137012 7.01379265
H -2.50137471 -0.92207831 7.79977086
S 0.99725315 -3.37479862 6.08671301
Fe 1.00043688 0.01396551 -2.23952733
Fe 1.02807517 -0.20085270 2.85930267
S 4.26540766 0.81314534 0.32021427
C -1.93759727 -1.49377793 0.28393699
H -1.95616552 -3.56679309 0.32360730
H -2.89342485 -0.84128190 -1.46884922
H -3.10644747 -0.76171110 1.85525513

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Listing S5. HC

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27
HS, Energy = -5076.012745 H
C -2.28190831 -2.62210518 -7.76955353
H -2.56284663 -0.56787565 -7.85553475
H -4.03818994 -3.47510426 -7.05136733
H -1.94432387 -3.35920341 -9.69484777
S 0.40213316 -3.31569812 -5.65738597
C 1.57606301 3.29373354 -7.35844928
H 3.42391523 3.96597767 -6.68727406
H 1.01832504 4.44632529 -9.00859059
H 1.79096721 1.31185662 -7.93261306
S -0.79847573 3.47813910 -4.81583865
C -2.08354987 5.15638282 2.93197739
H -1.21863646 5.12371124 1.05214145
H -2.16709842 7.13010952 3.60467260
H -4.02585861 4.45405403 2.73259777
S -0.27975217 3.16867996 5.15203571

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C	-1.59027439	-3.03107071	8.07979081
H	-1.89832095	-0.98326605	8.17172587
H	-0.97425784	-3.72263174	9.95295889
H	-3.40997359	-3.94032514	7.63279479
S	0.79130768	-3.71820521	5.62317417
Fe	-0.03478993	-0.25266009	-2.35732660
Fe	0.26452015	-0.52658586	2.52302989
S	3.94044001	0.17720368	-0.16367398
C	-2.57249201	-1.25056306	0.19231189
H	3.82334645	2.70489675	0.20264152
H	-4.27428958	-0.05798262	0.40347862
H	-3.11427509	-3.26422004	0.14094785

Listing S6. HS

27			
HFe, Energy = -5076.012745 H			
C	-3.75913157	-2.73243516	-5.62379855
H	-3.29406598	-0.86937361	-6.40698422
H	-5.34465440	-2.50613889	-4.30508511
H	-4.33389115	-4.02169448	-7.16164635
S	-0.94169345	-3.95902372	-4.00566722
C	3.36704638	0.78931871	-6.64033009
H	5.16356944	0.74240615	-5.59643989
H	3.70490535	1.68962586	-8.49608837
H	2.74508794	-1.16929167	-6.92812697
S	0.93491439	2.49051761	-4.84940786
C	-1.68456058	7.18270902	2.40049702
H	0.19224944	6.49260250	1.86699529
H	-1.50677428	9.06394023	3.29003486
H	-2.79670363	7.39397233	0.65959374
S	-3.19217575	4.89925564	4.56992044
C	-2.19692263	-4.80564329	4.43881601
H	-2.57539687	-4.92192958	2.40602069
H	-3.03292045	-6.46935583	5.38725653
H	-0.13958047	-4.84884165	4.68075772
S	-3.48483113	-1.83709967	5.73824166
Fe	0.38826032	-0.59158352	-1.35560261
Fe	-1.70350676	1.07471666	2.92488570
S	2.41535463	0.66757931	2.06352051
C	-3.11193692	0.30561124	-0.38195714
H	2.67456217	-2.54093001	-1.48834688
H	-3.80956887	2.12943289	-1.11041352
H	-4.60333594	-1.13690125	-0.42009557

Listing S7. HFe

27			
HFe2, Energy = -5076.012745 H			
C	-1.10308696	-3.43573011	-8.31015755
H	-1.97612529	-1.55868177	-8.47300817
H	-2.14811060	-4.78815975	-9.50868326
H	0.84450816	-3.32220378	-9.04341854
S	-1.16558991	-4.42709801	-4.97779147
C	1.01349275	2.98702318	-6.87382013
H	2.38288989	3.07635358	-5.32040867
H	1.08693632	4.76165870	-7.96939213
H	1.55847962	1.42276663	-8.12966587
S	-2.15634240	2.50020374	-5.54907517
C	-1.11945035	5.29777671	3.59413326
H	0.39205944	5.04544188	2.19778930
H	-0.71668237	6.96183152	4.78580215
H	-2.88709716	5.63793316	2.56070368
S	-1.34233521	2.43107787	5.53953962
C	-0.81834672	-3.19565308	8.30207207
H	-2.35902855	-1.86830822	8.70843936
H	0.96112552	-2.20397624	8.69784276
H	-0.97571351	-4.81794673	9.60760604
S	-0.94162510	-4.27161064	4.99428938
Fe	-1.11154921	-0.67337271	-2.32791573
Fe	-0.91042029	-0.60040006	2.27934685

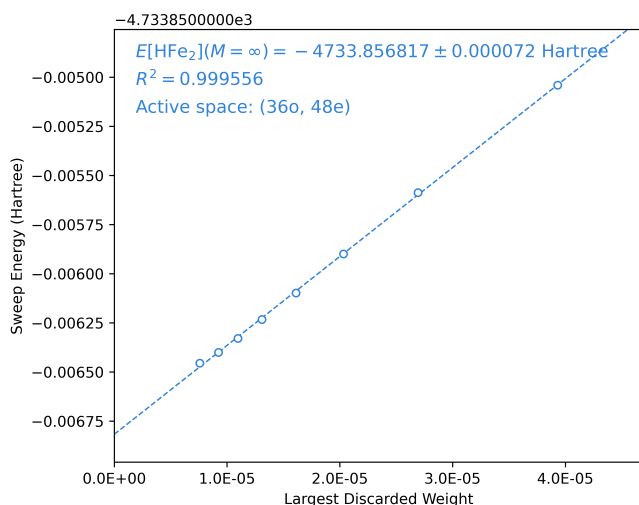
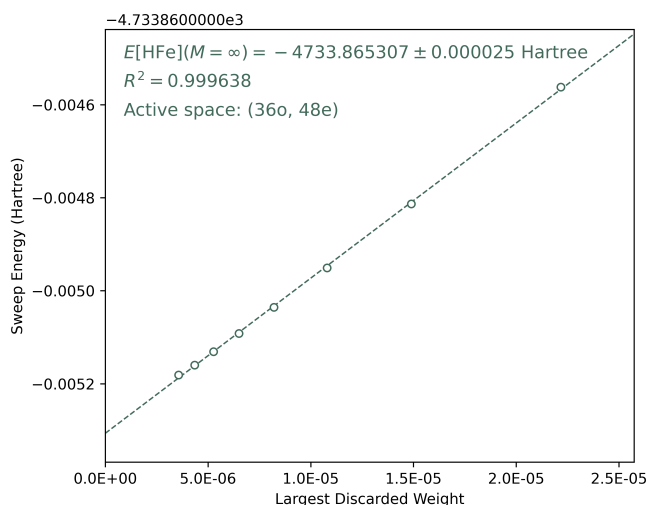
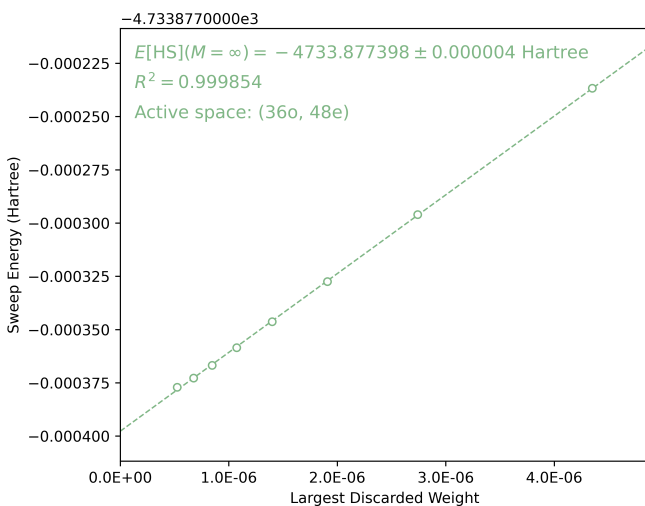
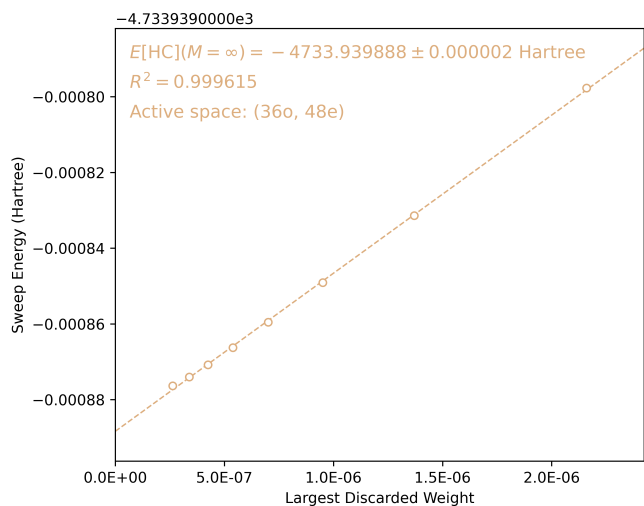
S	2.47213018	0.49721313	-0.26094746
C	-3.82542178	0.21332099	0.05633629
H	-1.08992756	-2.97599580	-0.02897393
H	-4.34227128	2.22216152	0.00023204
H	-5.46245532	-1.03979771	0.28218450

Listing S8. HFe₂

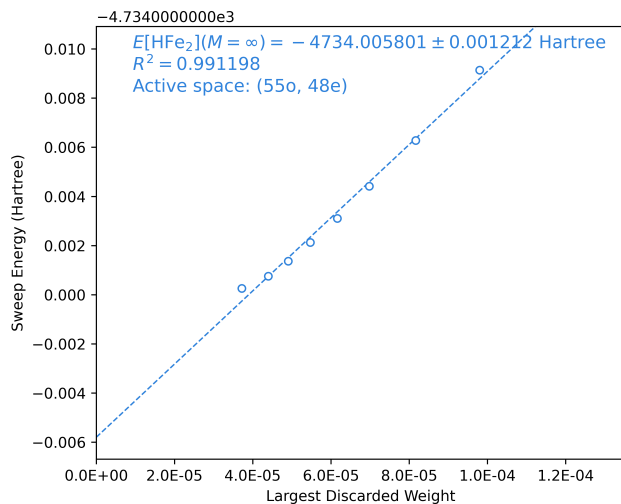
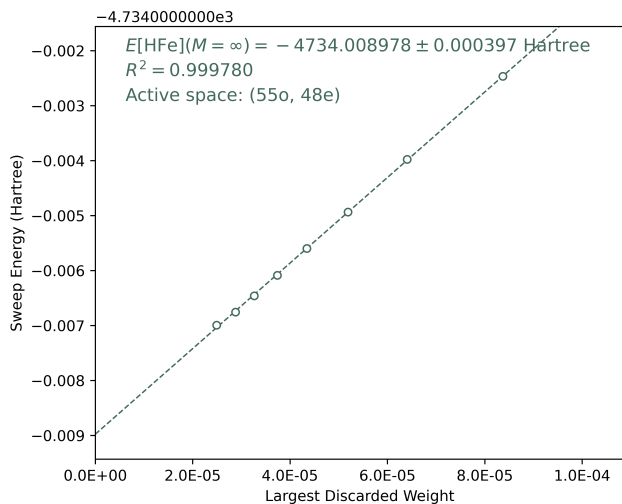
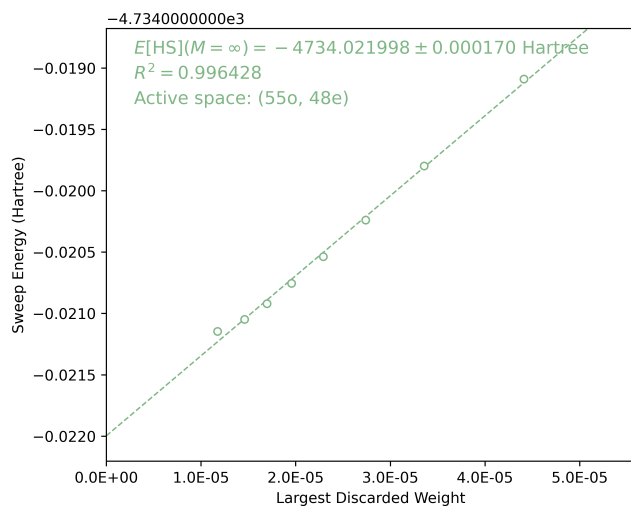
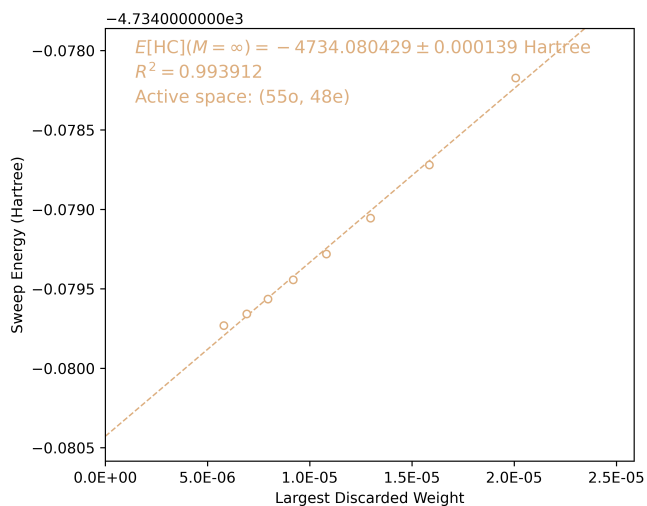
II. DMRG ENERGY EXTRAPOLATIONS

The following figures show the DMRG energy extrapolation process for the four protonated structures HC, HS, HFe, and HFe₂ in the (36o, 48e), (55o, 48e), and (63o, 64e) active spaces.

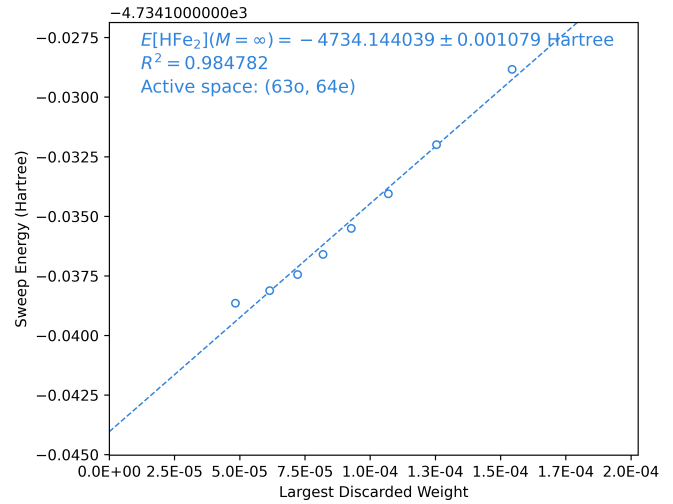
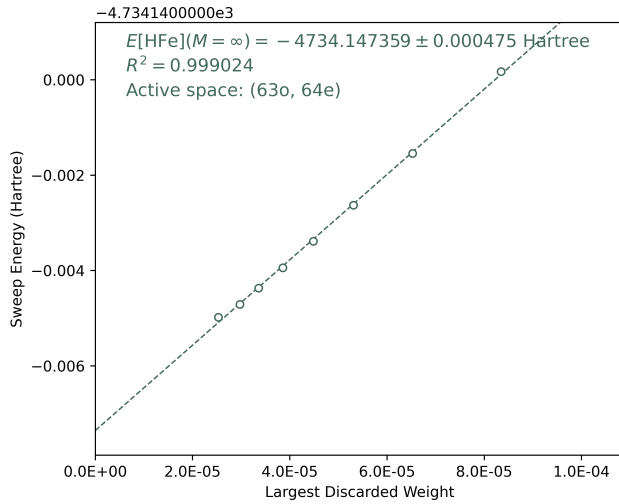
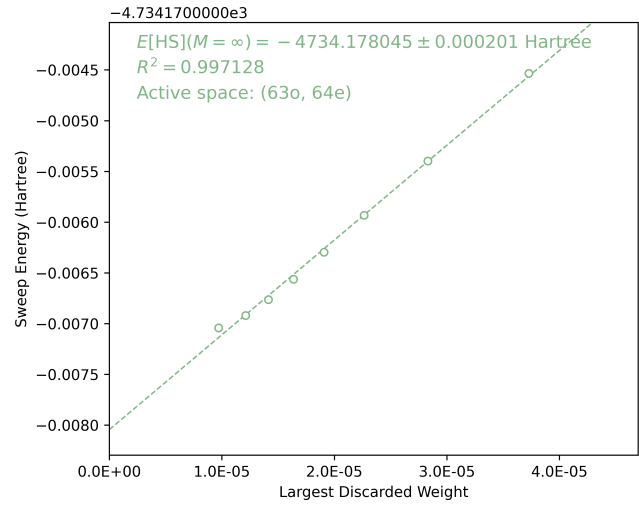
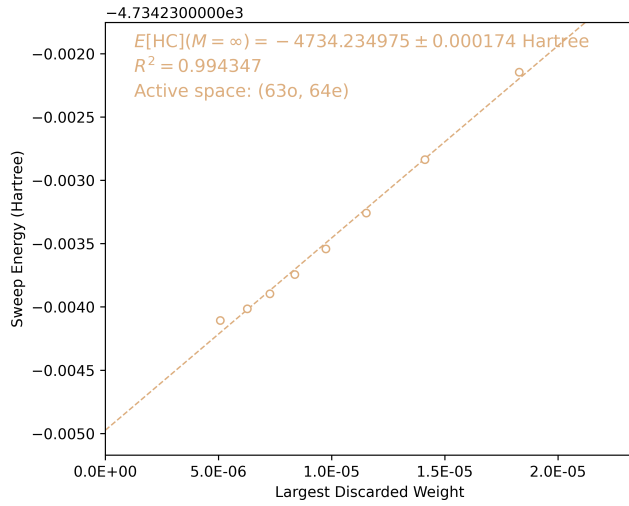
A. The (36o, 48e) active space



B. The (55o, 48e) active space



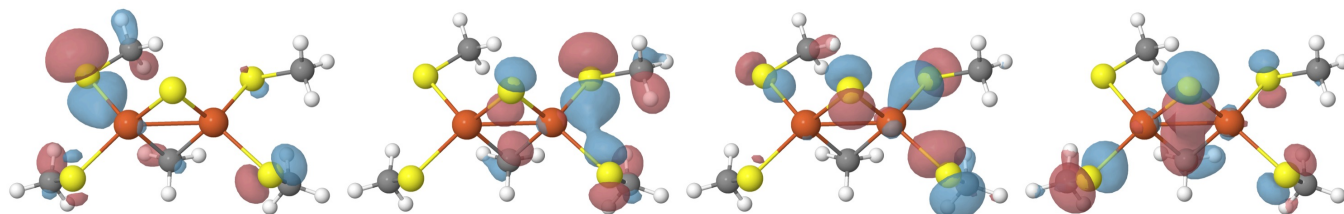
C. The (63o, 64e) active space



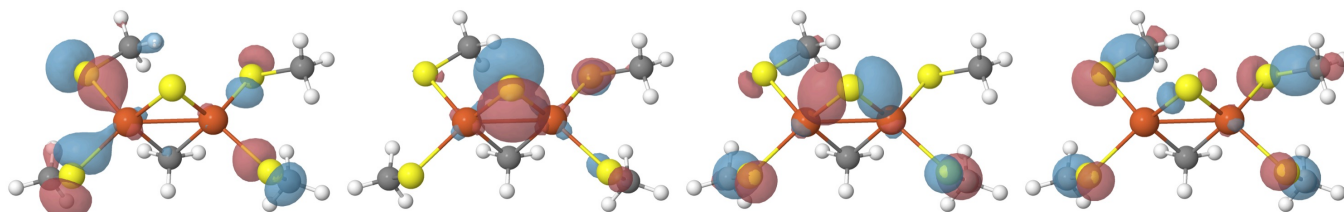
III. CCSD NATURAL ORBITALS

The following figures show the CCSD natural orbitals for constructing the active space. Orbitals are ordered according to the CCSD natural occupation number from highest to lowest, counting from zero. Orbital #86~#93 are close to singly occupied. The (36o, 48e) active space consists orbitals #66~#101. The (55o, 48e) active space consists orbitals #66~#120. The (63o, 64e) active space consists orbitals #58~#120.

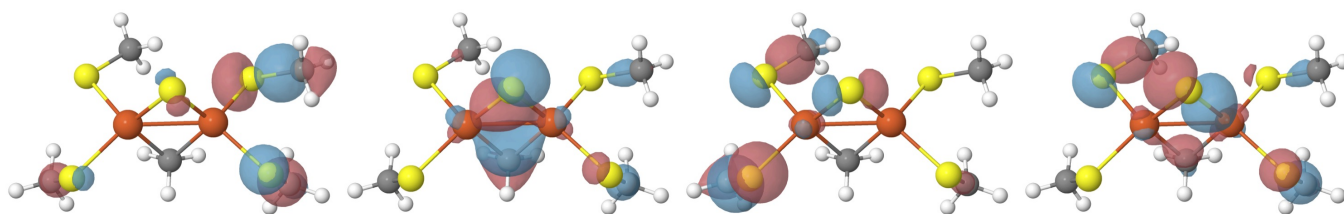
[HC- 77] occ = 1.948



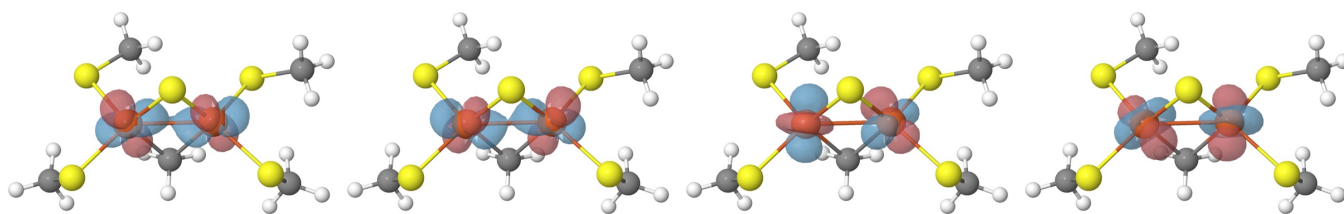
[HC- 81] occ = 1.943



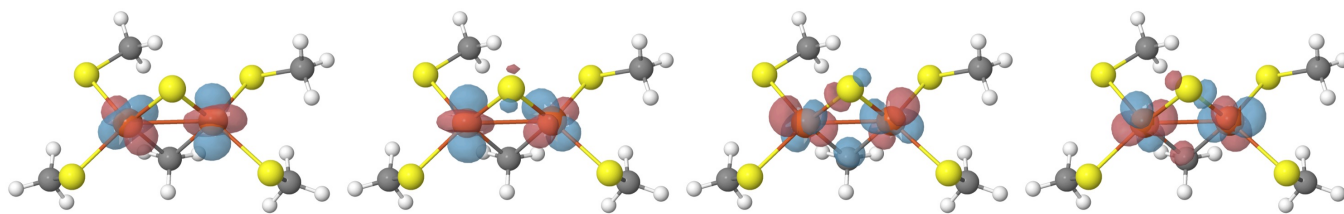
[HC- 85] occ = 1.941



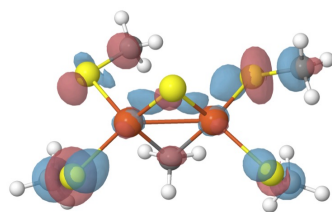
[HC- 89] $\text{occ} = 1.021$



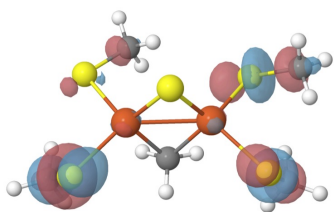
[HC- 93] $occ = 0.833$



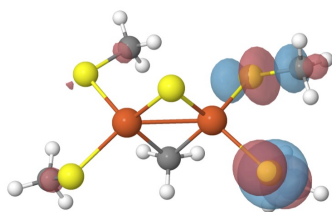
[HC- 94] occ = 0.051



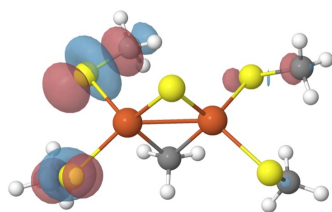
[HC- 95] occ = 0.048



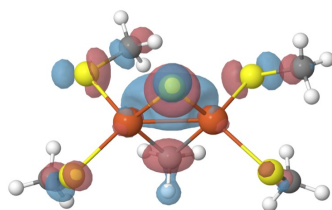
[HC- 96] occ = 0.044



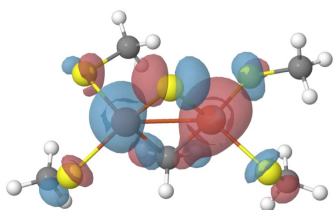
[HC- 97] occ = 0.044



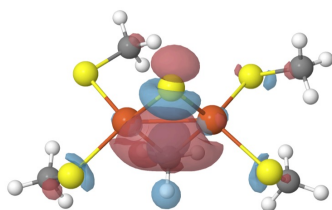
[HC- 98] occ = 0.038



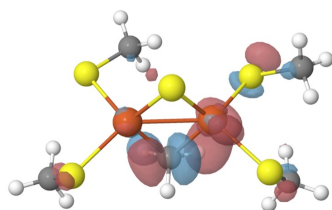
[HC- 99] occ = 0.032



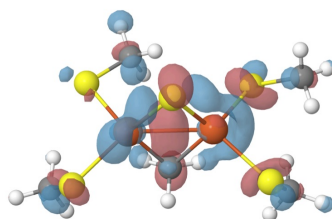
[HC-100] occ = 0.031



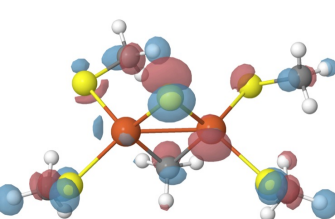
[HC-101] occ = 0.029



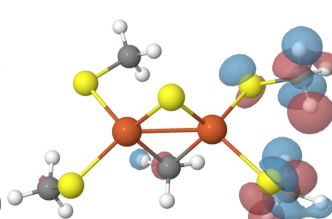
[HC-102] occ = 0.028



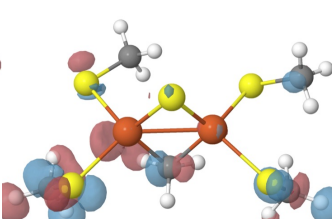
[HC-103] occ = 0.028



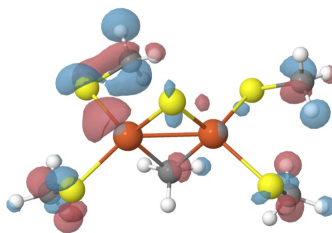
[HC-104] occ = 0.027



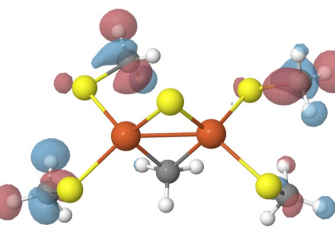
[HC-105] occ = 0.027



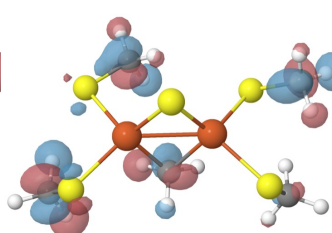
[HC-106] occ = 0.027



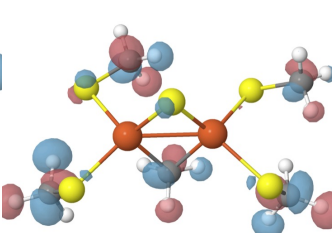
[HC-107] occ = 0.026



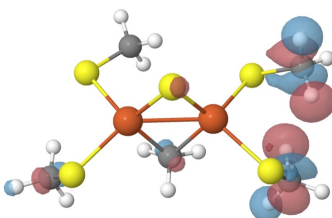
[HC-108] occ = 0.026



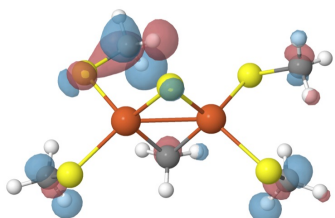
[HC-109] occ = 0.026



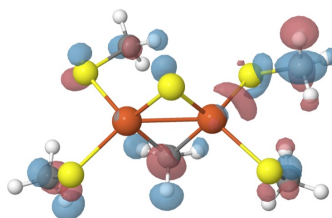
[HC-110] occ = 0.025



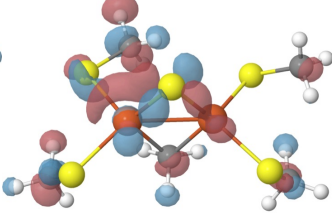
[HC-111] occ = 0.025



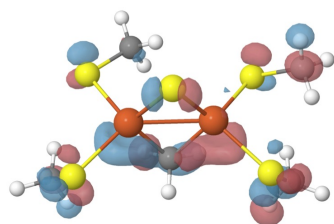
[HC-112] occ = 0.025



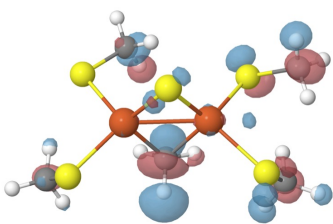
[HC-113] occ = 0.024



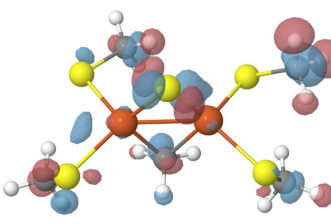
[HC-114] occ = 0.024



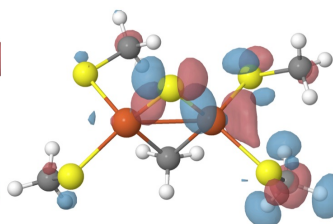
[HC-115] occ = 0.023



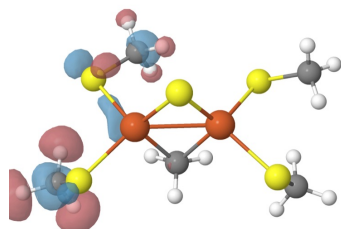
[HC-116] occ = 0.022



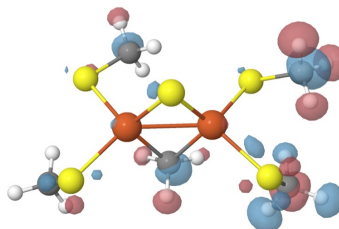
[HC-117] occ = 0.022



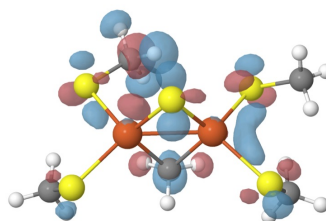
[HC-118] occ = 0.022



[HC-119] occ = 0.021

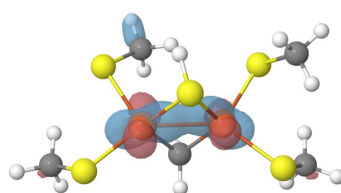


[HC-120] occ = 0.021

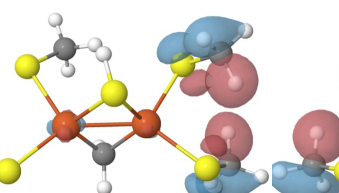


B. HS

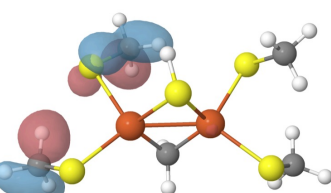
[HS- 58] occ = 1.961



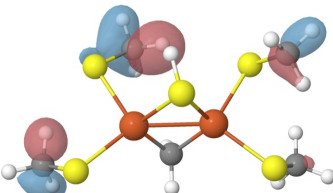
[HS- 59] occ = 1.961



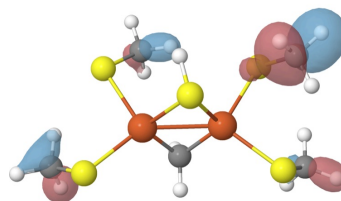
[HS- 60] occ = 1.960



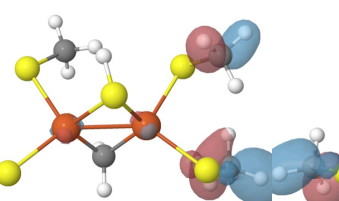
[HS- 61] occ = 1.959



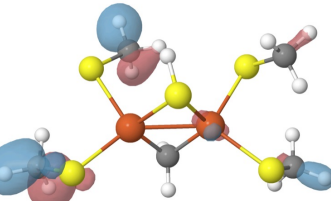
[HS- 62] occ = 1.958



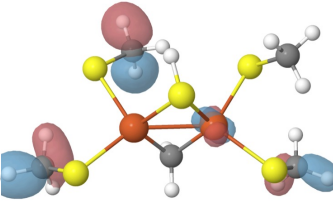
[HS- 63] occ = 1.958



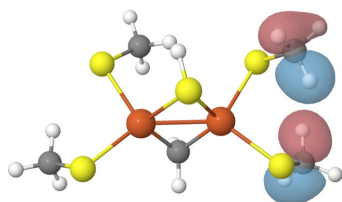
[HS- 64] occ = 1.958



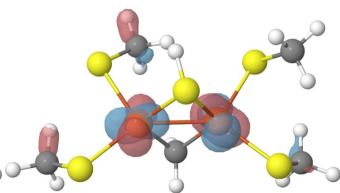
[HS- 65] occ = 1.958



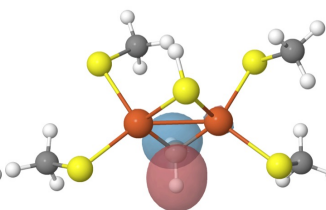
[HS- 66] occ = 1.958



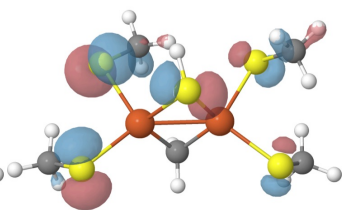
[HS- 67] occ = 1.957



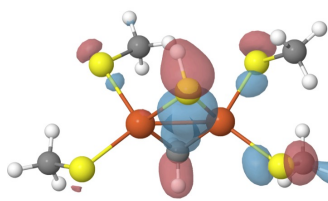
[HS- 68] occ = 1.955



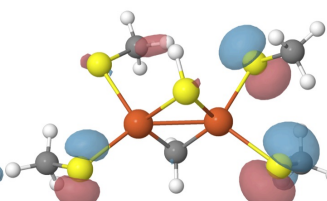
[HS- 69] occ = 1.952



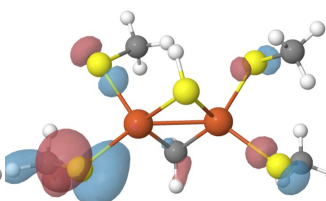
[HS- 70] occ = 1.951



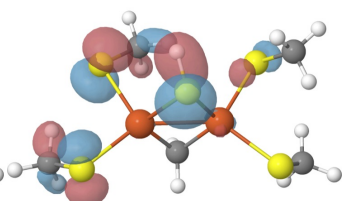
[HS- 71] occ = 1.951



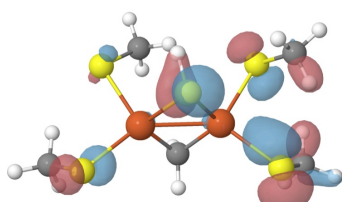
[HS- 72] occ = 1.950



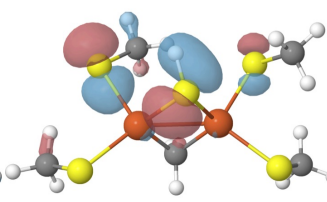
[HS- 73] occ = 1.950



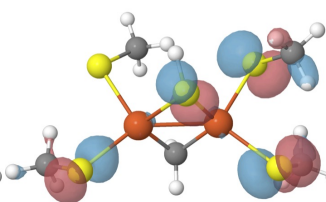
[HS- 74] occ = 1.949



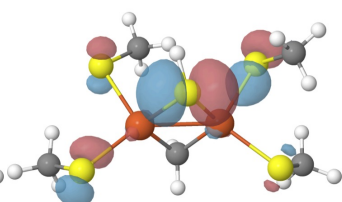
[HS- 75] occ = 1.949



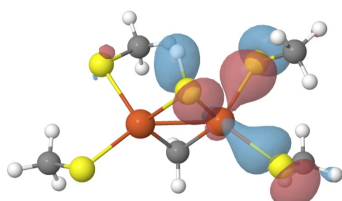
[HS- 76] occ = 1.949



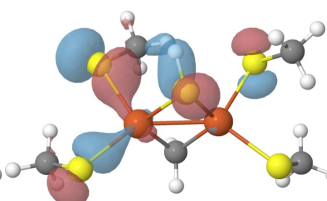
[HS- 77] occ = 1.948



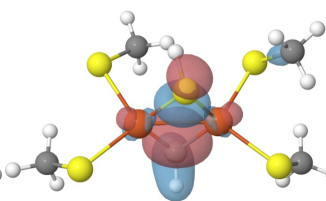
[HS- 78] occ = 1.947



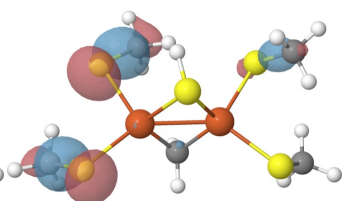
[HS- 79] occ = 1.947



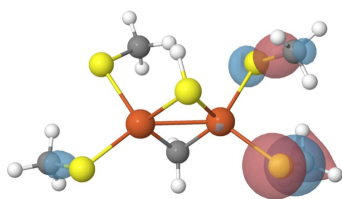
[HS- 80] occ = 1.944



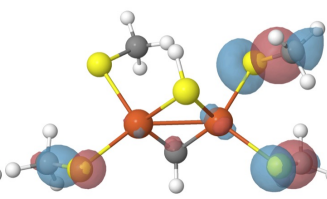
[HS- 81] occ = 1.943



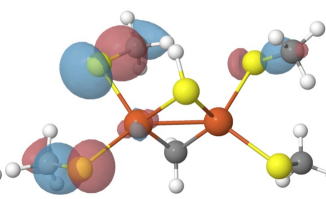
[HS- 82] occ = 1.943



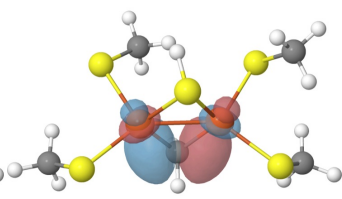
[HS- 83] occ = 1.942



[HS- 84] occ = 1.942



[HS- 85] occ = 1.924

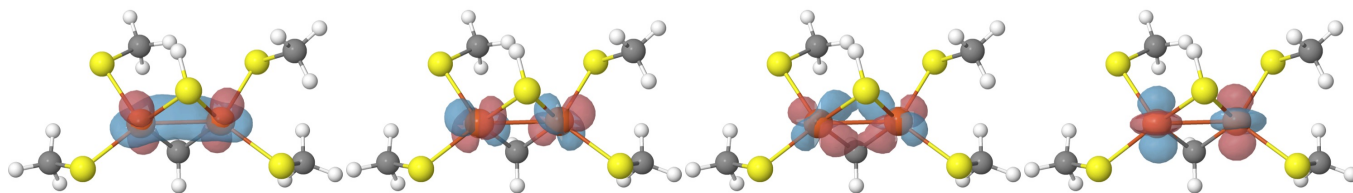


[HS- 86] occ = 1.317

[HS- 87] occ = 1.103

[HS- 88] occ = 1.089

[HS- 89] occ = 0.998

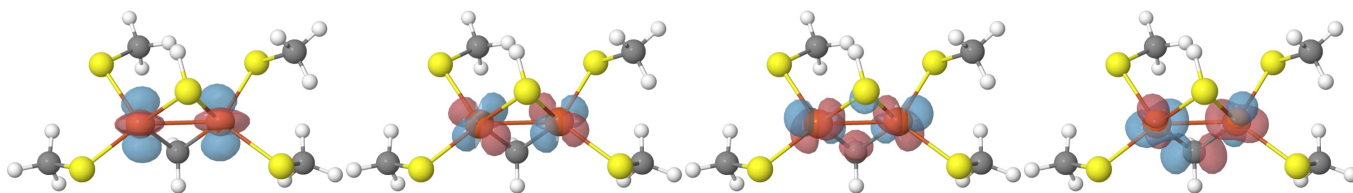


[HS- 90] occ = 0.991

[HS- 91] occ = 0.900

[HS- 92] occ = 0.891

[HS- 93] occ = 0.685

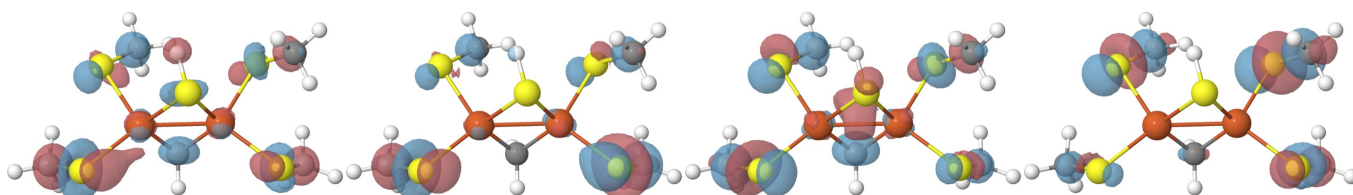


[HS- 94] occ = 0.052

[HS- 95] occ = 0.049

[HS- 96] occ = 0.046

[HS- 97] occ = 0.045

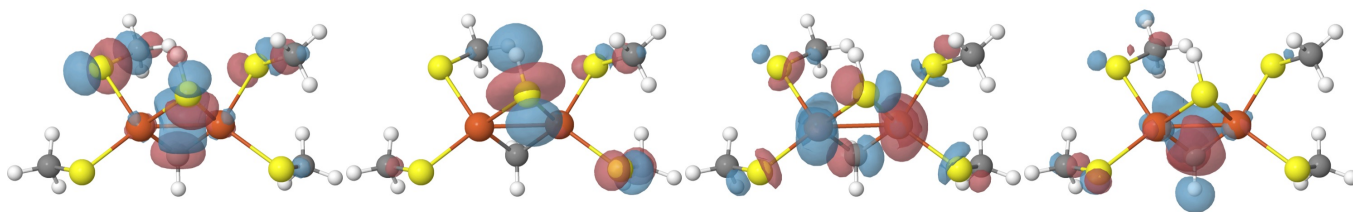


[HS- 98] occ = 0.042

[HS- 99] occ = 0.040

[HS-100] occ = 0.033

[HS-101] occ = 0.031

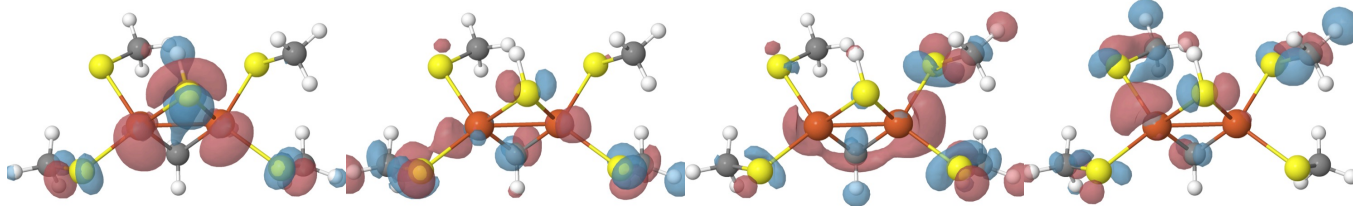


[HS-102] occ = 0.029

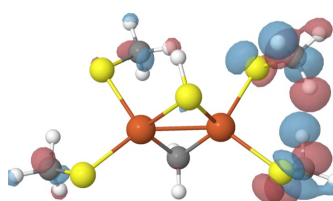
[HS-103] occ = 0.028

[HS-104] occ = 0.028

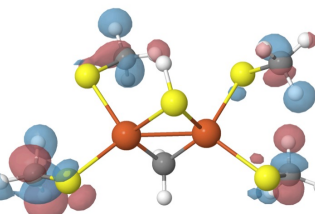
[HS-105] occ = 0.027



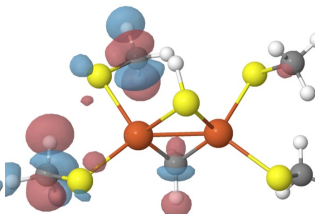
[HS-106] occ = 0.027



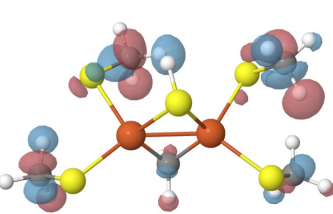
[HS-107] occ = 0.026



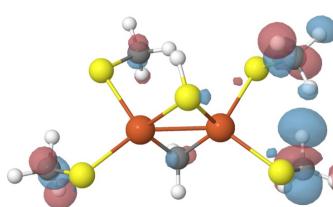
[HS-108] occ = 0.026



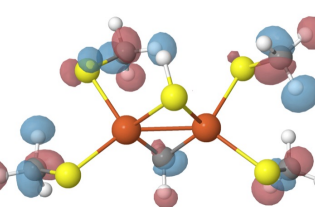
[HS-109] occ = 0.026



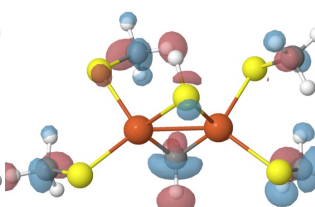
[HS-110] occ = 0.026



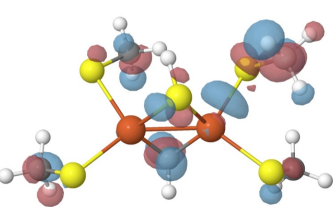
[HS-111] occ = 0.026



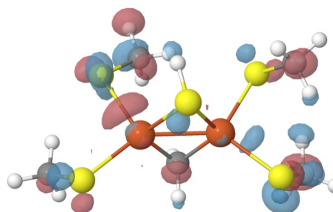
[HS-112] occ = 0.025



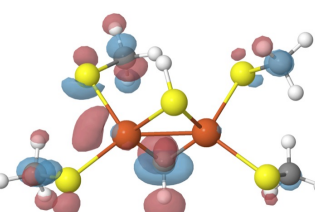
[HS-113] occ = 0.024



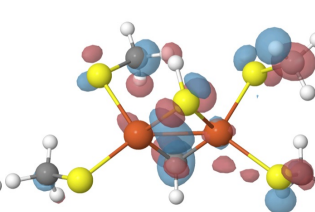
[HS-114] occ = 0.024



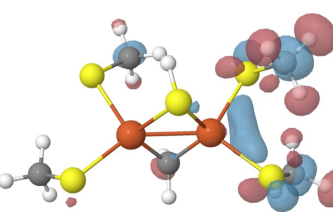
[HS-115] occ = 0.024



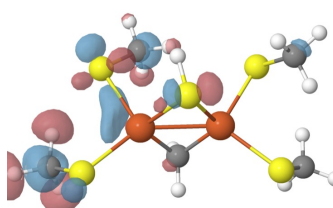
[HS-116] occ = 0.023



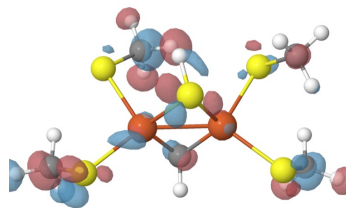
[HS-117] occ = 0.022



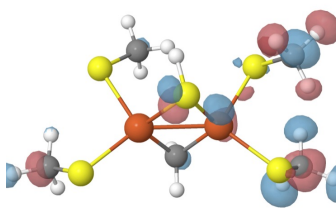
[HS-118] occ = 0.022

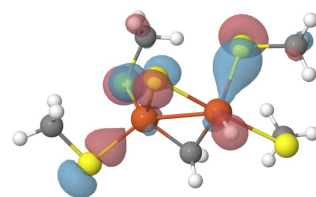


[HS-119] occ = 0.021

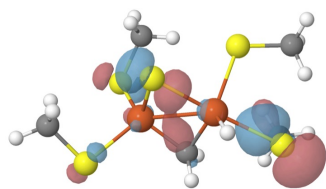


[HS-120] occ = 0.021

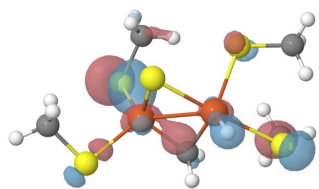




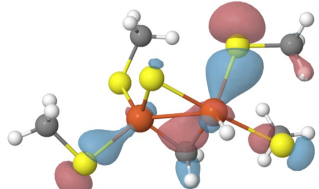
[HFe- 74] occ = 1.947



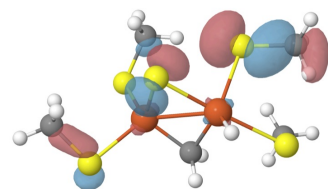
[HFe- 75] occ = 1.946



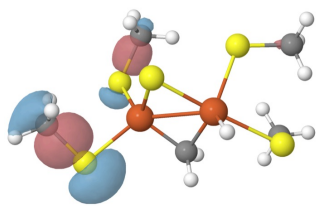
[HFe- 76] occ = 1.945



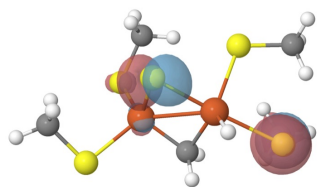
[HFe- 77] occ = 1.944



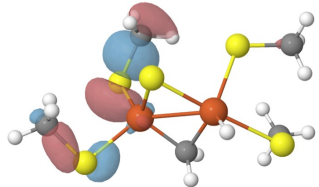
[HFe- 78] occ = 1.943



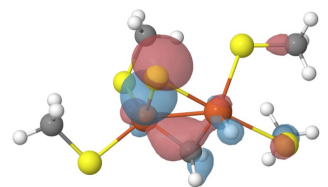
[HFe- 79] occ = 1.943



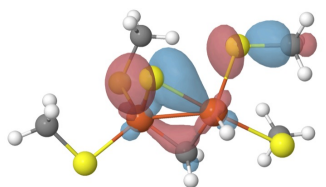
[HFe- 80] occ = 1.942



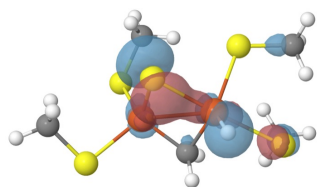
[HFe- 81] occ = 1.940



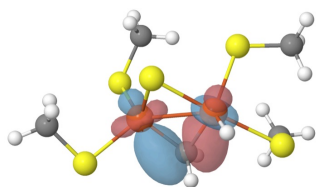
[HFe- 82] occ = 1.939



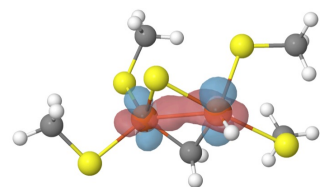
[HFe- 83] occ = 1.938



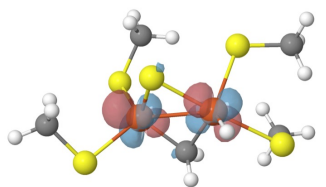
[HFe- 84] occ = 1.921



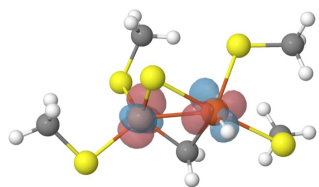
[HFe- 85] occ = 1.470



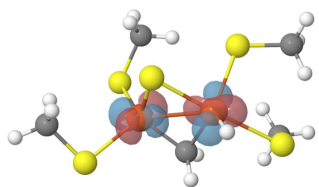
[HFe- 86] occ = 1.236



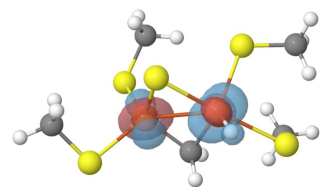
[HFe- 87] occ = 1.073



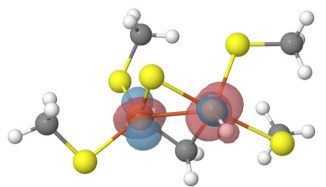
[HFe- 88] occ = 1.026



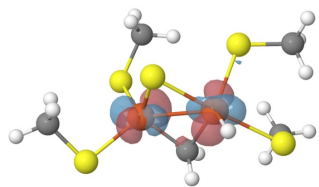
[HFe- 89] occ = 1.015



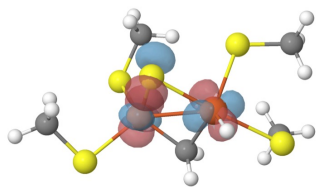
[HFe- 90] occ = 0.985



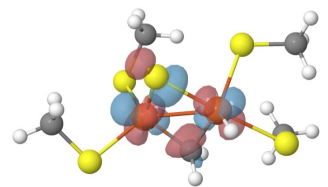
[HFe- 91] occ = 0.970



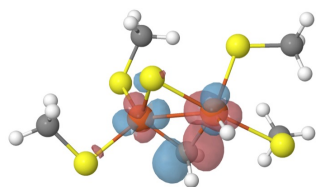
[HFe- 92] occ = 0.928



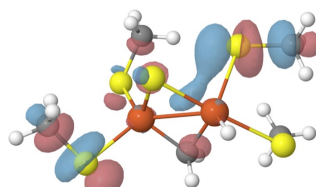
[HFe- 93] occ = 0.773



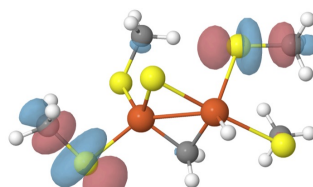
[HFe- 94] occ = 0.551



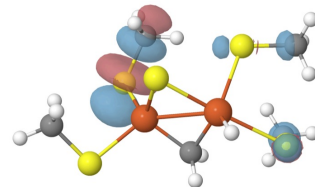
[HFe- 95] occ = 0.046



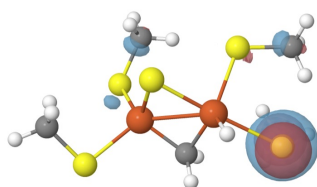
[HFe- 96] occ = 0.045



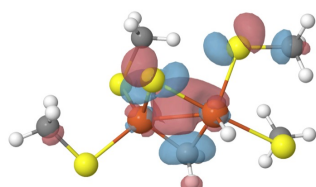
[HFe- 97] occ = 0.044



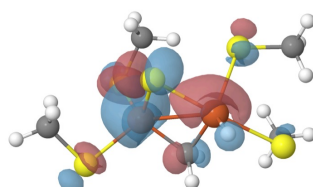
[HFe- 98] occ = 0.044



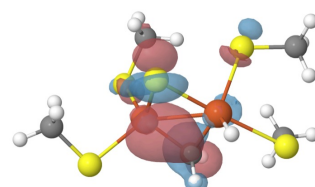
[HFe- 99] occ = 0.040



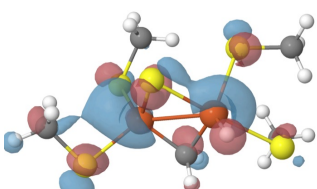
[HFe-100] occ = 0.032



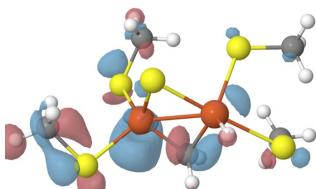
[HFe-101] occ = 0.031



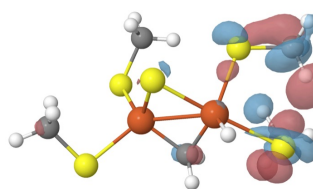
[HFe-102] occ = 0.030



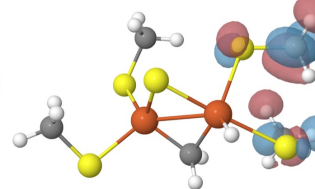
[HFe-103] occ = 0.028



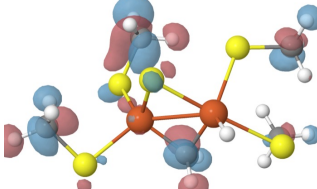
[HFe-104] occ = 0.028



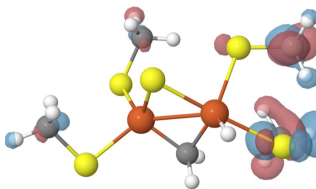
[HFe-105] occ = 0.027



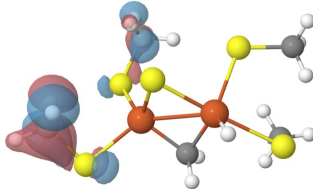
[HFe-106] occ = 0.026



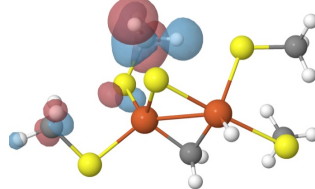
[HFe-107] occ = 0.026



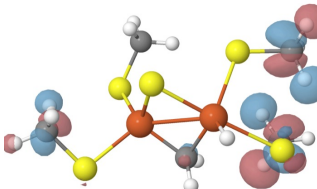
[HFe-108] occ = 0.026



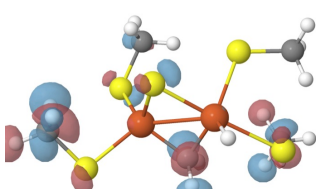
[HFe-109] occ = 0.026



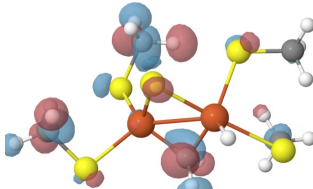
[HFe-110] occ = 0.025



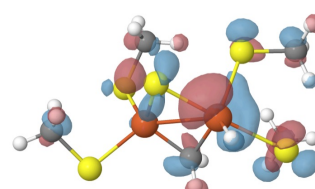
[HFe-111] occ = 0.025



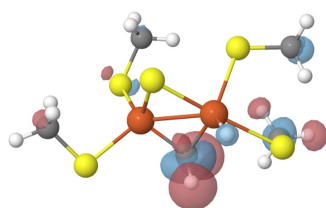
[HFe-112] occ = 0.025



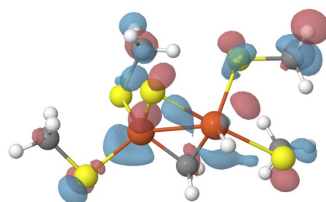
[HFe-113] occ = 0.024



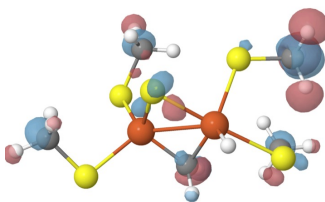
[HFe-114] occ = 0.023



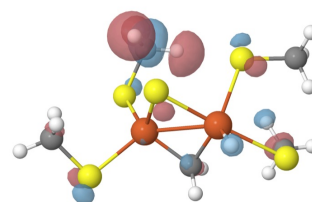
[HFe-115] occ = 0.023



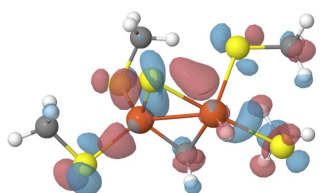
[HFe-116] occ = 0.023



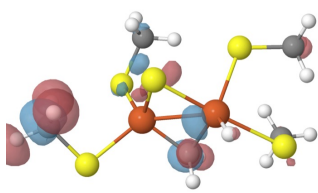
[HFe-117] occ = 0.022



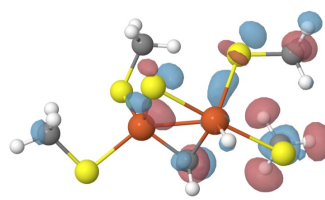
[HFe-118] occ = 0.022



[HFe-119] occ = 0.022

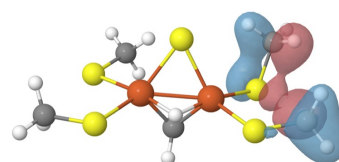


[HFe-120] occ = 0.021

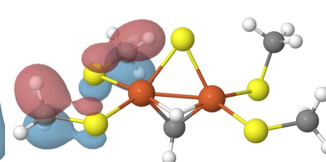


D. HFe₂

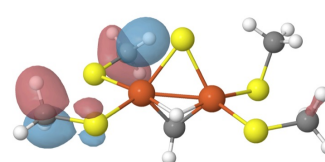
[HFe2- 58] occ = 1.960



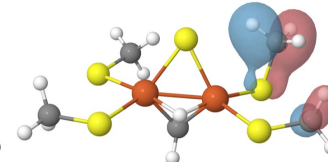
[HFe2- 59] occ = 1.960



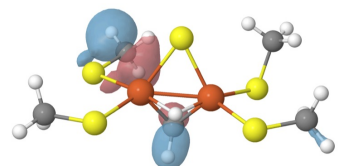
[HFe2- 60] occ = 1.959



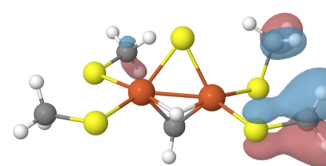
[HFe2- 61] occ = 1.959



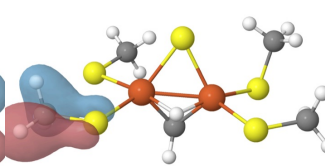
[HFe2- 62] occ = 1.959



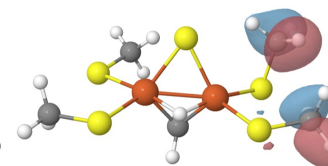
[HFe2- 63] occ = 1.959



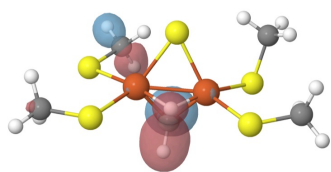
[HFe2- 64] occ = 1.958



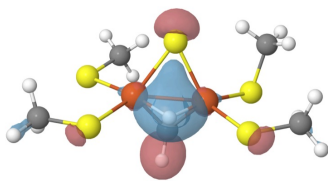
[HFe2- 65] occ = 1.957



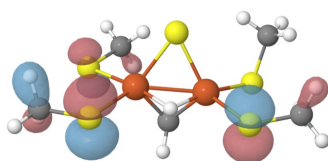
[HFe2- 66] occ = 1.956



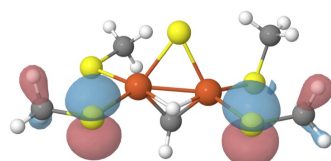
[HFe2- 67] occ = 1.954



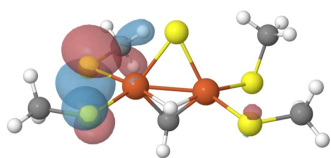
[HFe2- 68] occ = 1.951



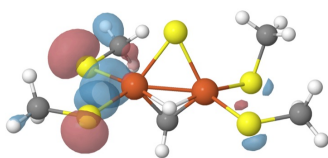
[HFe2- 69] occ = 1.951



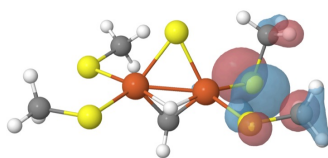
[HFe2- 70] occ = 1.951



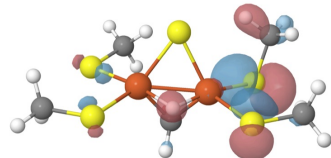
[HFe2- 71] occ = 1.950



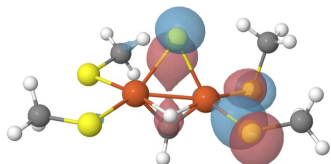
[HFe2- 72] occ = 1.949



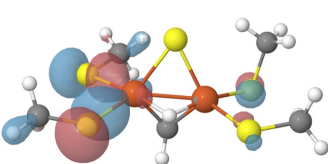
[HFe2- 73] occ = 1.949



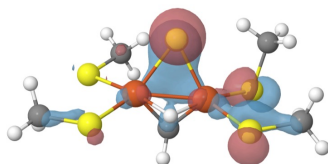
[HFe2- 74] occ = 1.948



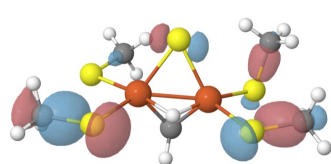
[HFe2- 75] occ = 1.947



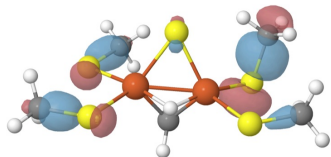
[HFe2- 76] occ = 1.946



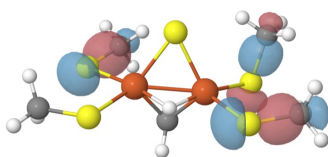
[HFe2- 77] occ = 1.944



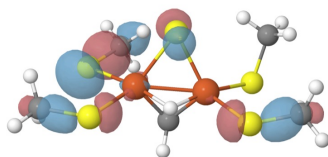
[HFe2- 78] occ = 1.943



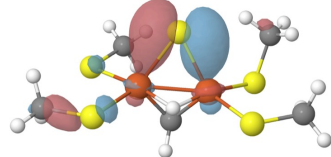
[HFe2- 79] occ = 1.943



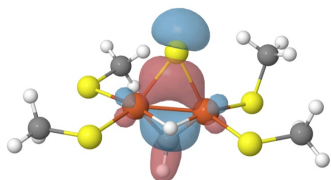
[HFe2- 80] occ = 1.942



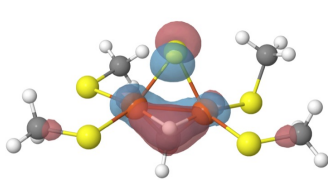
[HFe2- 81] occ = 1.941



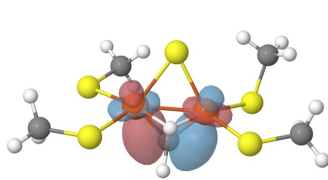
[HFe2- 82] occ = 1.939



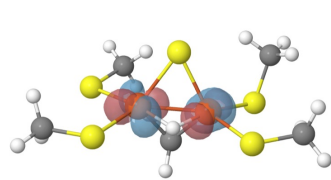
[HFe2- 83] occ = 1.933



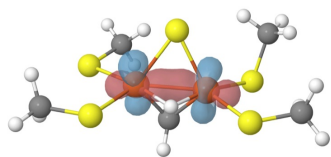
[HFe2- 84] occ = 1.919



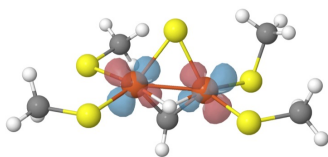
[HFe2- 85] occ = 1.532



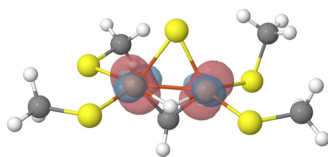
[HFe2- 86] occ = 1.486



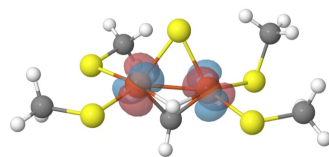
[HFe2- 87] occ = 1.212



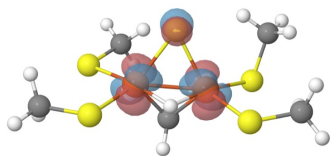
[HFe2- 88] occ = 1.030



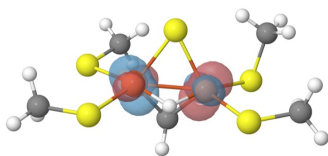
[HFe2- 89] occ = 1.019



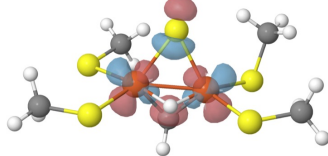
[HFe2- 90] occ = 0.978



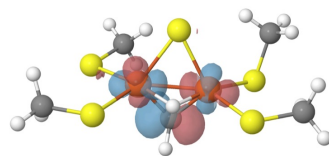
[HFe2- 91] occ = 0.962



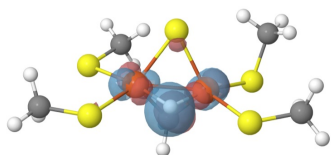
[HFe2- 92] occ = 0.793



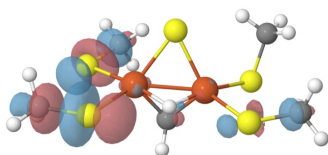
[HFe2- 93] occ = 0.534



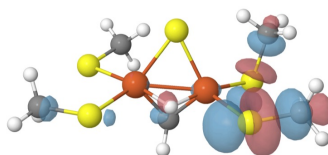
[HFe2- 94] occ = 0.487



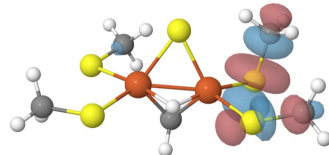
[HFe2- 95] occ = 0.047



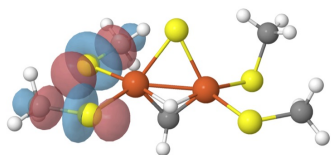
[HFe2- 96] occ = 0.045



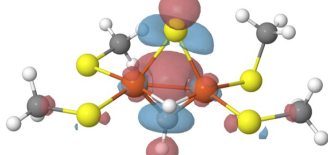
[HFe2- 97] occ = 0.044



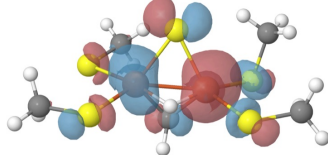
[HFe2- 98] occ = 0.044



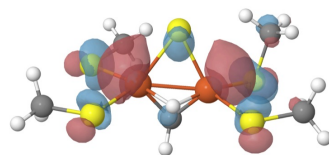
[HFe2- 99] occ = 0.036



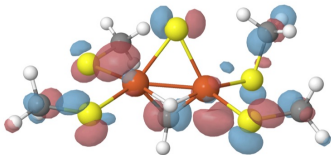
[HFe2-100] occ = 0.034



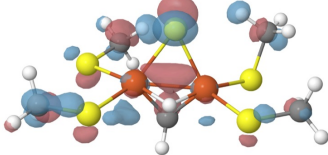
[HFe2-101] occ = 0.029



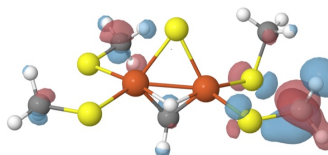
[HFe2-102] occ = 0.029



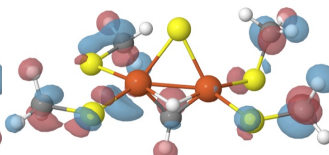
[HFe2-103] occ = 0.027



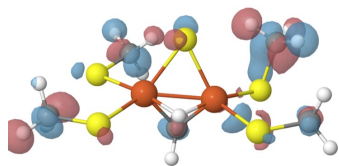
[HFe2-104] occ = 0.027



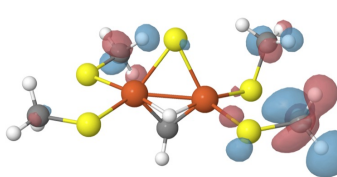
[HFe2-105] occ = 0.027



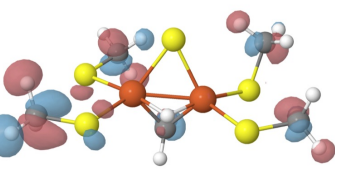
[HFe2-106] occ = 0.027



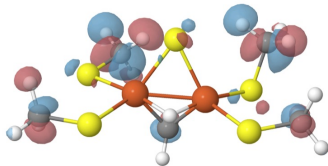
[HFe2-107] occ = 0.026



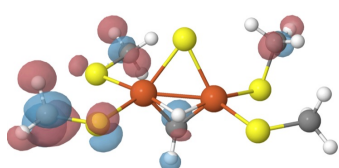
[HFe2-108] occ = 0.026



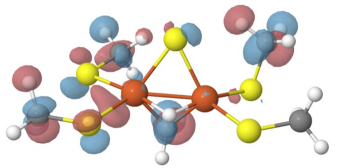
[HFe2-109] occ = 0.026



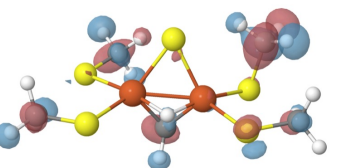
[HFe2-110] occ = 0.026



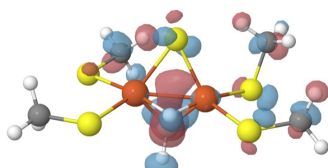
[HFe2-111] occ = 0.026



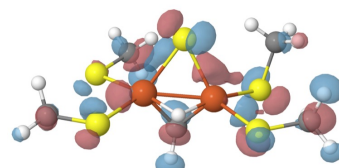
[HFe2-112] occ = 0.025



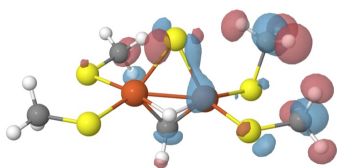
[HFe2-113] occ = 0.024



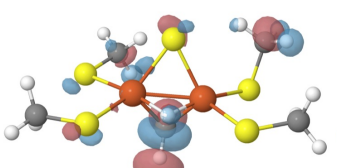
[HFe2-114] occ = 0.024



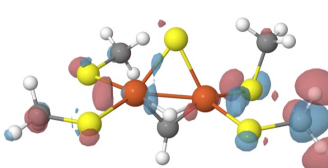
[HFe2-115] occ = 0.023



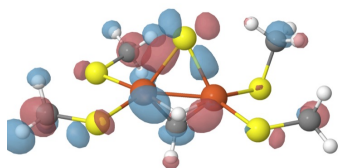
[HFe2-116] occ = 0.023



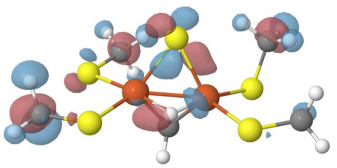
[HFe2-117] occ = 0.022



[HFe2-118] occ = 0.022



[HFe2-119] occ = 0.022



[HFe2-120] occ = 0.021

