SUPPORTING INFORMATION
of
Density Functional Theory Study of an All Ferrous 4Fe-4S Cluster

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Decomposition of BS M_S = 4 state (II in Figure 2) in terms of proper cluster spin states:

$$|M_{1-3} = 6, M_4 = -2, M_S = 4\rangle = \sum_{S=4}^{8} C_S |\{S_{1-3} = 6, S_4 = 2\} S, M_S = 4\rangle$$

The moduli and squares of the expansion coefficients are given in following table:

Expansion of BS M_S = 4 in pure spin states

S	$\lvert C_S \rvert$	C_S^2
4	0.832	0.692
5	0.492	0.242
6	0.239	0.057
7	0.091	0.008
8	0.023	0.001

Optimized geometry in the BS M_S = 4 state (II in Figure 2)

Fe	0.590685	0.169731	1.131776
Fe	1.810722	-1.108396	2.931825
Fe	0.555542	-2.379398	1.097003
Fe	-0.814166	-1.093936	2.955277
S	0.470718	0.724019	3.369041
S	0.419954	-2.896559	3.374047
S	-1.334126	-1.042429	0.782289
S	2.607280	-1.147844	0.605893
C	-2.404857	-1.182354	4.038934
C	3.694965	-1.216625	3.723450
C	0.962706	-3.896456	-0.240343
C	1.022349	1.624783	-0.237848
C	-4.526351	-0.879892	4.881085
C	-3.880943	-1.740845	5.715084
C	5.609684	-1.318673	4.976484
C	5.976375	-1.311555	3.660936
C	2.213138	-4.966126	-1.824710
C	1.092813	-5.720172	-1.620139
C	1.157259	3.435120	-1.634413
C	2.244131	2.644051	-1.876200
N	-2.603418	-1.905225	5.191078
N	-3.615786	-0.552076	3.880964
N	4.800546	-1.248710	2.935087
N	4.221522	-1.259925	4.983457
N	2.101842	-3.877529	-0.979266
N	0.354287	-5.047147	-0.654523
N	0.434786	2.792107	-0.636817
N	2.132379	1.564839	-1.018321
H	-5.532112	-0.481005	4.919362
H	-4.218709	-2.233563	6.617978
H	6.206568	-1.358046	5.879440
H	6.958266	-1.344906	3.205457
H	3.053001	-5.122189	-2.490288
H	0.773355	-6.651913	-2.070642
H	0.851297	4.374741	-2.077642
H	3.062905	2.770107	-2.573582
H	-1.881906	-2.522050	5.547538
H	-3.801223	0.042588	3.082890
H	4.651103	-1.230159	1.913811
H	3.640860	-1.250159	5.813227
H	2.740970	-3.078438	-0.836111
H	-0.537718	-5.351503	-0.283632
H	-0.432386	3.126469	-0.233885
H	2.752606	0.749105	-0.891398

Bond distances in the optimized BS M_S = 4 geometry. (Fe_4 is special iron)

	Distance (Å)
Fe_4-S_1	2.224
Fe_4-S_2	2.235
Fe_4-S_3	2.264
Fe_1-S_2	2.301
Fe_1-S_3	2.308
Fe_1-S_4	2.466
Fe_2-S_1	2.308
Fe_2-S_3	2.312
Fe_2-S_4	2.459
Fe_3-S_1	2.339
Fe_3-S_2	2.336
Fe_3-S_4	2.443
Fe_1-C_1	2.044
Fe_2-C_2	2.047
Fe_3-C_3	2.063
Fe_4-C_4	1.927

Bond angles in the optimized BS M_S = 4 geometry. (Fe_4 is special iron)

	Angle (°)
Fe_4-S_2-Fe_1	70.7
Fe_4-S_3-Fe_1	70.1
Fe_4-S_1-Fe_2	70.8
Fe_4-S_3-Fe_2	70.0
Fe_4-S_1-Fe_3	70.7
Fe_4-S_2-Fe_3	70.6
Fe_1-S_3-Fe_2	66.2
Fe_1-S_4-Fe_2	61.6
Fe_1-S_2-Fe_3	66.7
Fe_1-S_4-Fe_3	62.6
Fe_2-S_1-Fe_3	66.9
Fe_2-S_4-Fe_3	63.0