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Supplementary Information

Spin-Crossover in Cyanide-Based Bimetallic Coordination Polymers – Insight from First-Principles Study

Soumyajit Sarkar, Kartick Tarafder, Peter M. Oppeneer and Tanusri Saha-Dasgupta

	1Ag-HS-dh (2Ag-HS)	**1Ag-LS-dh(2Ag-LS)**
a	14.2138	11.9786
b	13.3136	13.2460
c	7.6334	8.8477
α	90.00	90.00
β	92.311	96.915
γ	90.00	90.00
Ag1	0.2554 0.7533 0.2638	0.2422 0.7465 0.2464
Ag2	0.2384 0.5660 0.0169	0.2531 0.5690 0.9913
Fe1	0.0000 0.5000 0.5000	0.0000 0.5000 0.5000
Fe2	0.5000 0.5000 0.5000	0.5000 0.5000 0.5000
N1	0.0908 0.6040 0.3836	0.0699 0.6083 0.4048
N2	0.0583 0.5471 0.7482	0.0729 0.5377 0.6960
N3	0.8887 0.6186 0.5111	0.8660 0.5885 0.5246
N4	0.7274 0.6709 0.4685	0.6650 0.5980 0.5108
N5	0.5829 0.3994 0.3757	0.5765 0.3754 0.4129
N6	0.4191 0.5217 0.2751	0.4458 0.5467 0.2758
C1	0.1498 0.6600 0.3366	0.1236 0.6660 0.3407
C2	0.1200 0.5602 0.8557	0.1295 0.5533 0.8134
C3	0.9148 0.7153 0.5399	0.8734 0.6880 0.5610
C4	0.8493 0.7931 0.5312	0.7771 0.7457 0.5708
C5	0.7553 0.7673 0.4945	0.6728 0.6977 0.5456
C6	0.7959 0.6012 0.4776	0.7614 0.5481 0.5004
C7	0.6396 0.3439 0.3190	0.6375 0.3234 0.3503
C8	0.3568 0.5375 0.1702	0.3805 0.5576 0.1648
H1	0.9896 0.7286 0.5687	0.9579 0.7198 0.5811
H2	0.8713 0.6293 0.0526	0.7840 0.6740 0.0979
H3	0.7001 0.8245 0.4851	0.5937 0.7371 0.5536
H4	0.2249 0.4770 0.5441	0.2447 0.5314 0.5293

Table 1: Theoretically optimized crystal structure of 1Ag-HS-dh and 1Ag-LS-dh compounds

	2Cu
a	11.4692
b	13.3232
c	8.0665
α	90.00
β	95.10
γ	90.00
Cu1	0.2492 0.7509 0.2504
Cu2	0.2516 0.5948 -0.0015
Fe1	0.0000 0.5000 0.5000
Fe2	0.5000 0.5000 0.5000
N1	0.0746 0.6073 0.3874
N2	0.0723 0.5483 0.7094
N3	0.8552 0.5884 0.5127
N4	0.6447 0.5876 0.4897
N5	0.5753 0.3932 0.3874
N6	0.4291 0.5489 0.2901
C1	0.1351 0.6678 0.3270
C2	0.1344 0.5727 0.8293
C3	0.8543 0.6906 0.5162
C4	0.7490 0.7435 0.5011
C5	0.6442 0.6898 0.4856
C6	0.7502 0.5416 0.5016
C7	0.6361 0.3331 0.3267
C8	0.3678 0.5730 0.1692
H1	0.9391 0.7278 0.5288
H2	0.7483 0.8252 0.5012
H3	0.5589 0.7260 0.4725
H4	0.7506 0.4606 0.5024

Table 2: Theoretically optimized crystal structure of 2Cu compound