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Origins of Contrasting Copper Coordination Geometries in Crystalline Copper Sulfate Pentahydrate

Michael T. Ruggiero[†], Alessandro Erba[‡], Roberto Orlando[‡], and Timothy M. Korter[†]*

[†] *Department of Chemistry, Syracuse University, 1-014 Center for Science and Technology, Syracuse, NY 13244-4100, United States*

[‡] *Dipartimento di Chimica and Centre of Excellence Nanostructured Interfaces and Surfaces, Università di Torino, via Giuria 5, IT-10125 Torino, Italy*

*tmkorter@syr.edu

Table S1: Experimental single-crystal XRD fractional atomic coordinates for $CuSO_4 \cdot 5H_2O$. The crystals have $P\bar{1}$ space group symmetry, and lattice dimensions of: *a* = 6.106 Å, *b* = 10.656 Å, *c* = 5.969 Å, α = 77.332°, β = 82.433°, γ = 72.523°, and *V*=360.548 Å^3

Atom	X/A	Y/B	Z/C
Cu	0.5000	1.0000	0.5000
Cu	0.5000	0.5000	1.0000
S	0.8741	0.5140	0.7140
O	0.7032	0.7469	0.6832
O	0.4804	1.2569	0.5826
O	0.7955	1.0345	0.4056
H	0.8400	1.1540	0.3820
H	0.9110	0.9250	0.3920
O	0.8257	0.4056	0.8488
O	0.3491	0.7900	0.8822
O	0.3522	0.3159	0.9257
H	0.2870	0.2300	0.9790
H	0.2600	0.3800	0.8690
O	1.1154	0.5431	0.6999
O	0.8632	0.3620	0.6264
O	0.1299	0.0679	0.1244
H	0.1650	-0.0760	0.1300
H	0.1940	0.0860	0.1840
H	0.3570	1.3420	0.6120
H	0.5830	1.2990	0.5920
H	0.2290	0.8150	0.8760
H	0.4290	0.8020	0.8070

Table S.2: Details of the experimental structure refinement of $CuSO_4 \cdot 5H_2O$.

Parameter	Value
Temperature	90 K
Radiation Type	Molybdenum K_α
F (0 0 0)	246
Crystal Size	0.21 x 0.14 x 0.10
Reflections Collected	21157
R indices ($I > 2\sigma(I)$)	R_1=0.0420, wR_2=0.0586
R indices (all data)	R_1=0.0607, wR_2=0.0627
Goodness-of-fit on F^2	1.016