



Supplementary Materials



Figure S1. (a) XANES spectra of Cu(II)Phen crystals and Mt-CuPhen compared with the spectra of several reference compounds: Cu₂O, CuO, CuS, CuSO₄·5H₂O, and Cu₃(CO₃)₂(OH)₂. (b) XANES spectra of Cu(II)Phen crystals and Mt-CuPhen compared with the CuO and CuSO₄·5H₂O references showing more clearly the XANES features of compounds. The insets present a zoom of the peaks related to the 1s \rightarrow 3d and 1s \rightarrow 4p transitions. (c) Smoothed first derivative of absorption signal of Cu(II)Phen crystals, Mt-CuPhen and reference compounds. The 1s \rightarrow 3d transition characteristics of Cu(II) compounds is marked by a dotted vertical line on Figure S1c.



Figure S2. XANES spectra of Mt-CuPhen exposed to H₂S gas under different conditions. (**a**) Mt-CuPhen exposed to H₂S for different times, i.e., 12 h, 5 d, 1 month, 2 months and (**b**) Mt-CuPhen exposed 12 h and 1 month to H₂S in aerobic and anaerobic conditions and Mt-CuPhen first exposed to H₂S for 1 month in anaerobic conditions and then exposed to air for 2 weeks.



Figure S3. Linear relationship between position at Cu *K*-absorption edge and the oxidation state for reference compounds, Cu(II)Phen crystals, Mt-CuPhen material and this last one exposed to H₂S gas under different conditions: (**a**) Mt-CuPhen exposed to H₂S for 12 h (Mt-CuPhen-exp H₂S-12h), 5 d (Mt-CuPhen-exp H₂S-5d), 1 month (Mt-CuPhen-exp H₂S-1m), 2 months (Mt-CuPhen-exp H₂S-2m) in aerobic conditions, (**b**) Mt-CuPhen exposed to H₂S in anaerobic conditions for 12 h (Mt-CuPhen-exp H₂S-2m) H₂S ac-12h), 1 month (Mt-CuPhen-exp H₂S ac-1m), and for 1 month and re-exposed to air (Mt-CuPhen-exp H₂S ac-1m-air).