Tetranuclear Copper(I) Carboxylate: The Effect of a Stepwise Increase in Lewis Acidity on Solid-State Structures

Oleksandr Hietsoi, Alexander S. Filatov, Cristina Dubceac, and Marina A. Petrukhina*

Department of Chemistry, University at Albany, State University of New York,

1400 Washington Avenue, Albany, New York 12222, USA

SUPPLEMENTARY INFORMATION

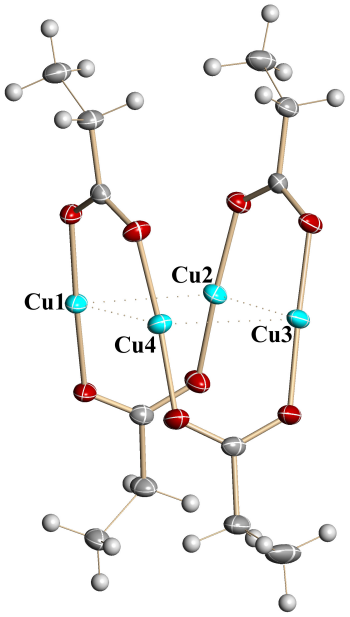

Fig. S1 Thermal ellipsoid representation (40% probability ellipsoids) of the $[Cu_4(O_2CCH_2CH_3)_4]$ (**1**) complex. Cu blue, O red, C grey, H light grey. This color scheme is used in all figures.

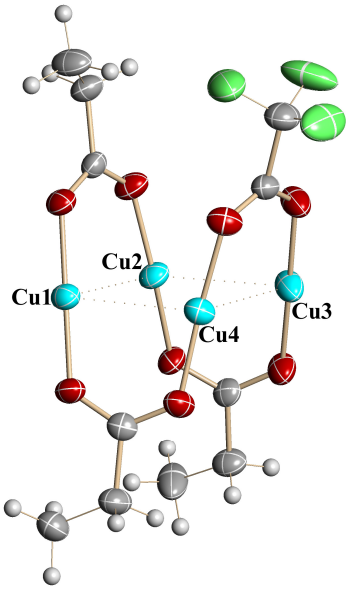

Fig. S2 Thermal ellipsoid representation (40% probability ellipsoids) of the $[Cu_4(O_2CCF_3)(O_2CCH_2CH_3)_3]$ (**2**) complex. Only one part of the rotationally disordered CF_3 group is shown.

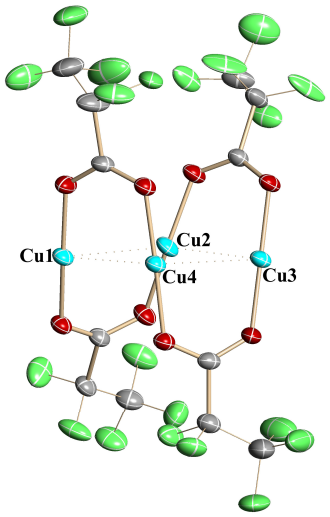

Fig. S3 Thermal ellipsoid representation (40% probability ellipsoids) of the $[Cu_4(O_2CCF_2CF_3)_4]$ (**3**) complex. Only major parts of the two disordered C_2F_5 groups are shown.

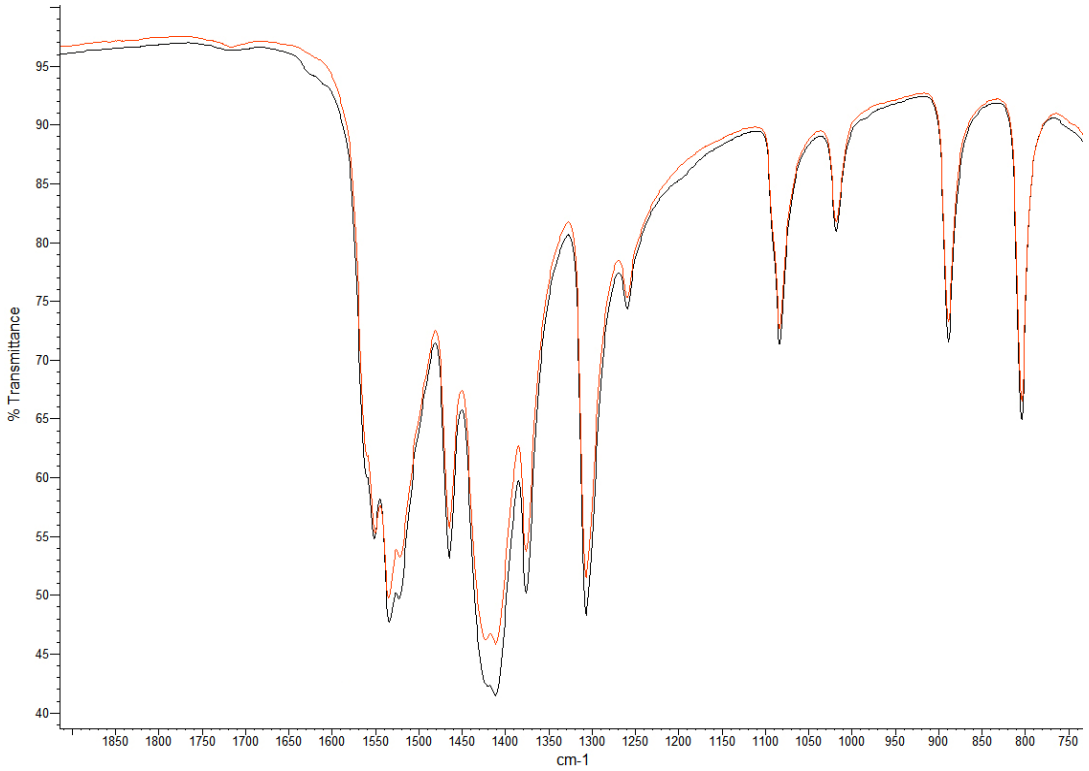

Fig. S4 IR spectra (carboxylate region) of copper(I) propionate obtained by Edwards's *et al.*, method (black) and of the microcrystalline bulk sample of **1** (red).

X-ray powder diffraction details

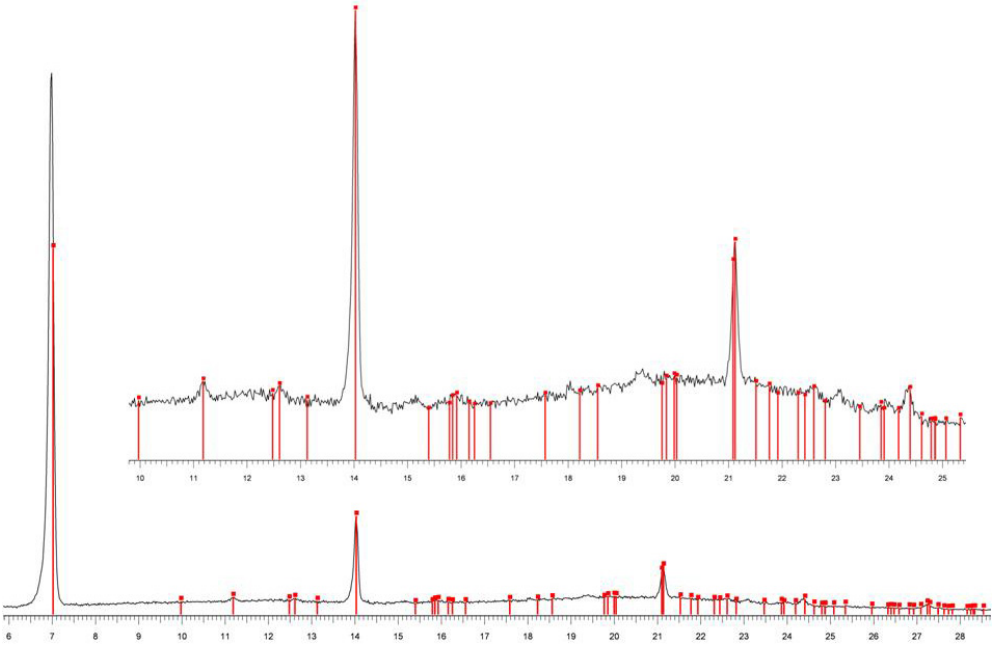

Fig. S5 The observed X-ray powder pattern for the bulk microcrystalline sample of **1** (black) *vs*. the simulated X-ray powder pattern based on the single crystal diffraction data of **1** (red).

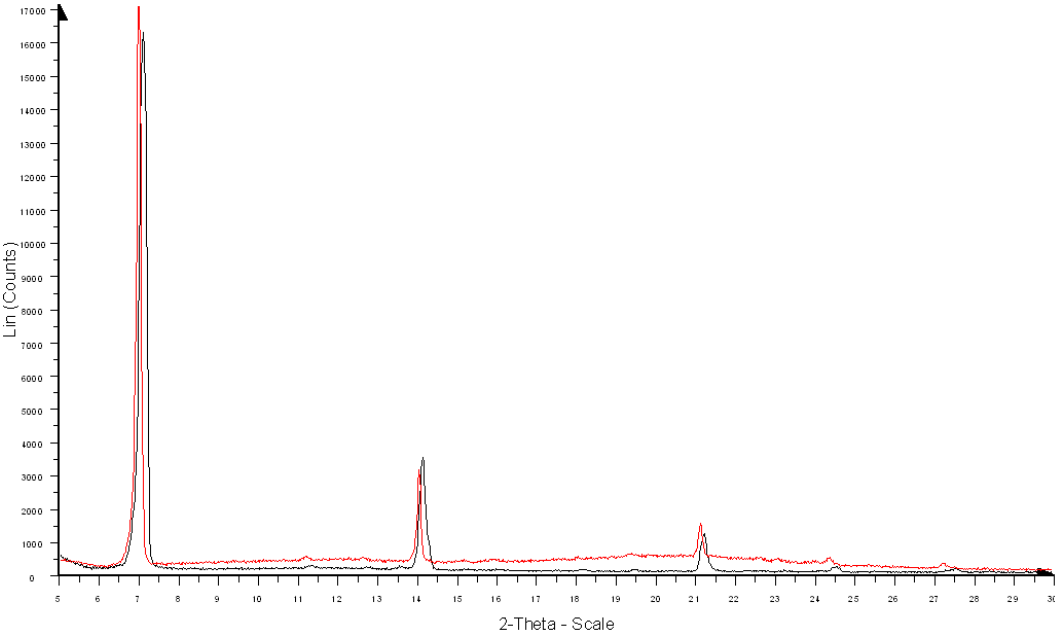

Fig. S6 The observed X-ray powder patterns for the bulk microcrystalline sample obtained by Edwards's *et al*., method (black) *vs*. bulk microcrystalline sample of **1** (red).

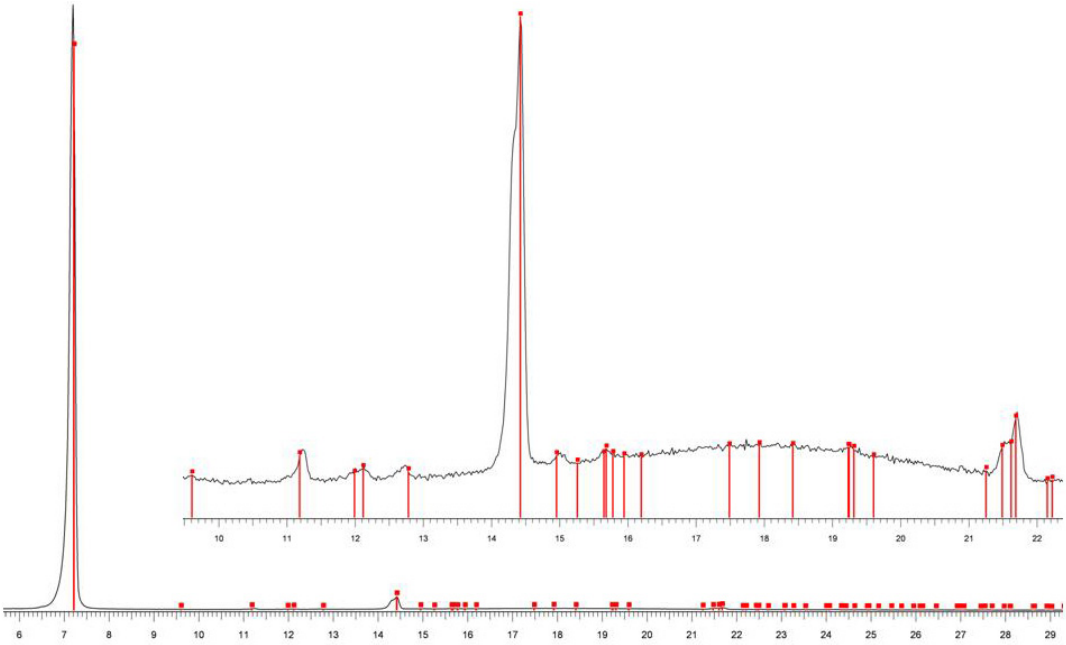

Fig. S7 The observed X-ray powder pattern for the bulk microcrystalline sample of **2** (black) *vs*. the simulated X-ray powder pattern based on the single crystal diffraction data of **2** (red).

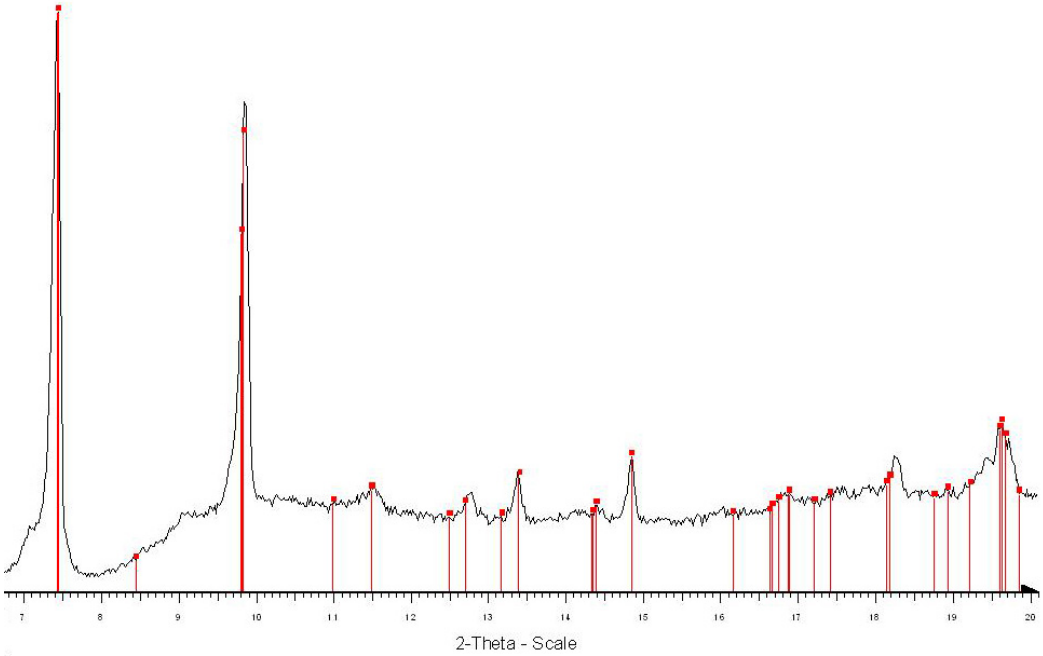

Fig. S8 The observed X-ray powder pattern for the single crystals of **3** (black) *vs*. the simulated X-ray powder pattern based on the single crystal diffraction data of **3** (red).