

Mono- and dinuclear copper(II) and iron(III) complexes of a tetradentate bispidine-diacetate ligand

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Accessory Publication

Table S1. Selected bond lengths (Å) and angles (°) for LH₂.

| | | | |
|-----------------|----------|-----------------|----------|
| C(13)-O(1) | 1.313(4) | C(15)-O(3) | 1.226(3) |
| C(13)-O(2) | 1.195(4) | C(15)-O(4) | 1.263(4) |
| N(3)-C(12) | 1.441(4) | N(7)-C(14) | 1.484(4) |
| N(3)···N(7) | 2.668 | | |
| O(1)-C(13)-O(2) | 123.8(3) | O(3)-C(15)-O(4) | 125.5(3) |

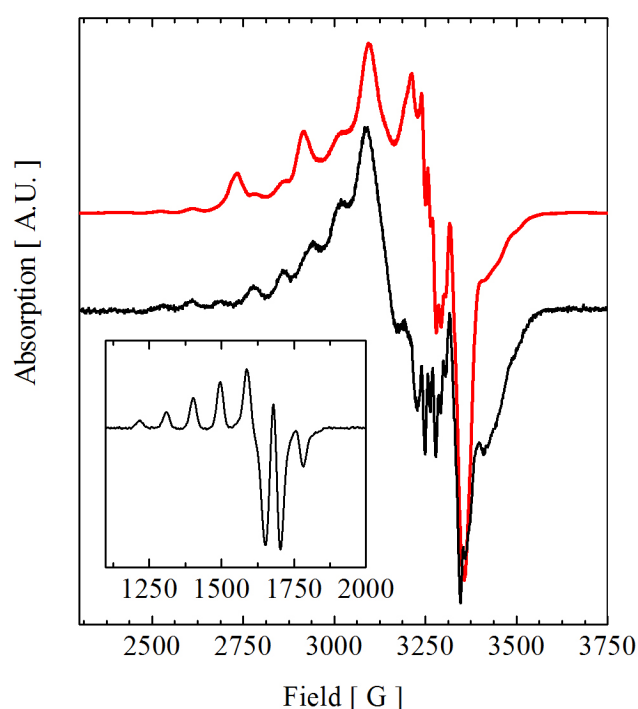


Figure S1. X-band EPR spectrum of **1** (red, top) measured in a 10 mM methanolic solution ($T = 6.4$ K, $\nu = 9.395996$ GHz) compared with the spectrum obtained after

subtraction of the signal due to the monomeric species. Inset shows the half-field signal observed with the 10mM methanolic solution.

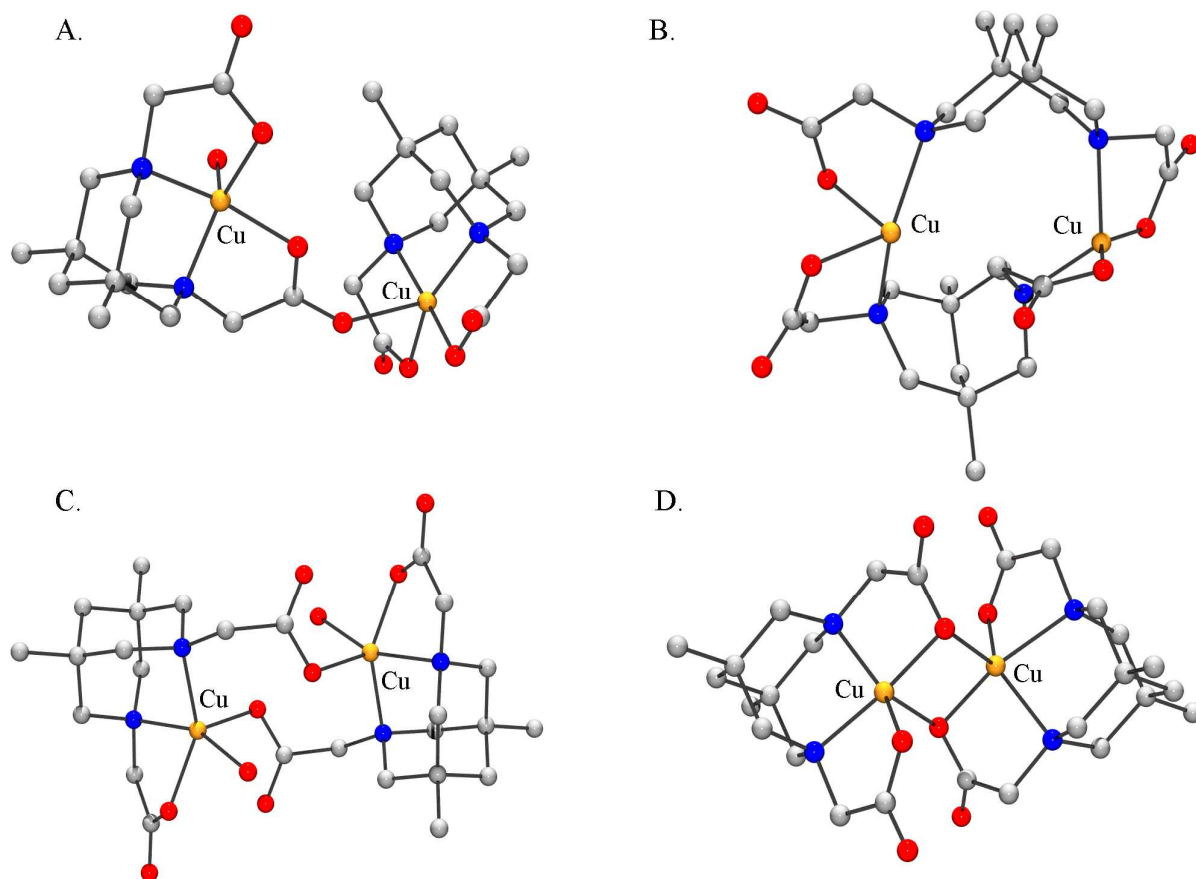


Figure S2. Possible structures of the dimeric species **1b**: A. type (a) with the single carboxylate bridge ($\text{Cu}\cdots\text{Cu} = 5.6 \text{ \AA}$); B. type (b) with the bridging bispidine ligand ($\text{Cu}\cdots\text{Cu} = 4.6 \text{ \AA}$); C. type (c) with one carboxylate cleaved at each centre and coordinated to the other Cu(II) ion ($\text{Cu}\cdots\text{Cu} = 5.2 \text{ \AA}$); D. type (d) with the diamond-like Cu_2O_2 motif ($\text{Cu}\cdots\text{Cu} = 2.99 \text{ \AA}$).

