

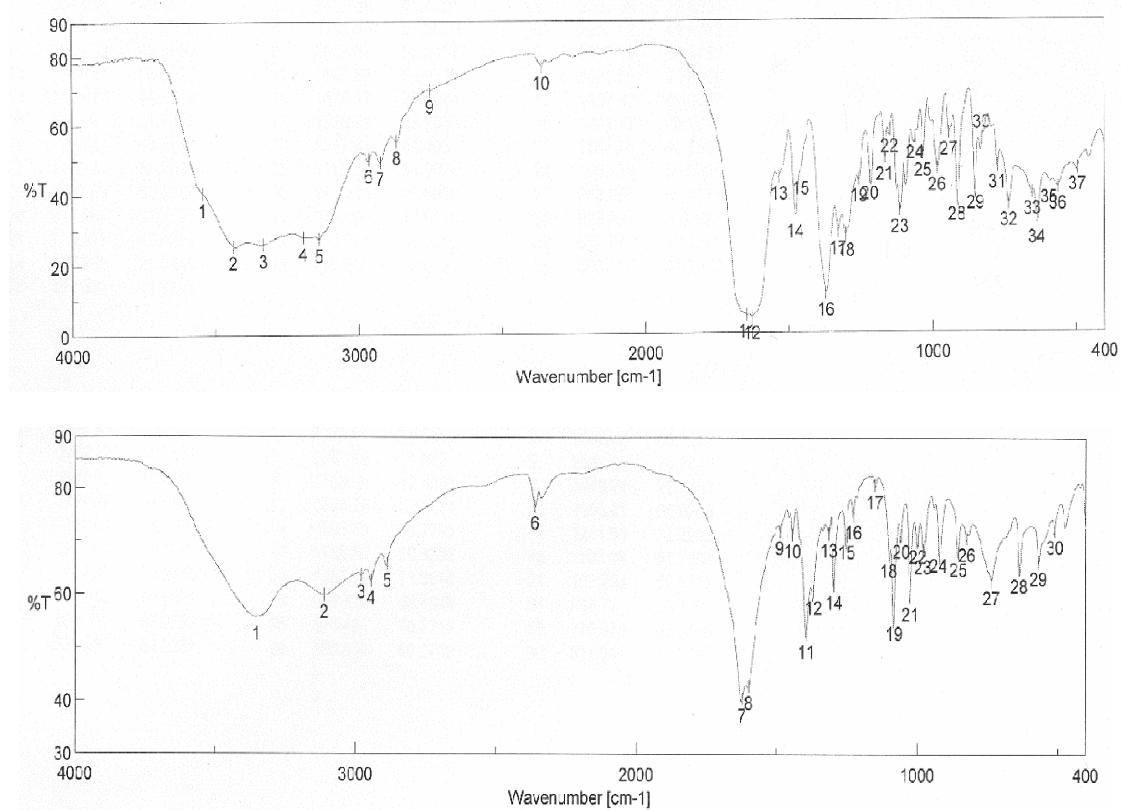
Supplementary Material for manuscript:

**H(N3)dap (Hdap = 2,6-Diaminopurine) Recognition  
by Cu<sub>2</sub>(EGTA): Structure, Physical Properties, and  
Density Functional Theory Calculations of [Cu<sub>4</sub>(μ-  
EGTA)<sub>2</sub>(μ-H(N3)dap)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]·7H<sub>2</sub>O**

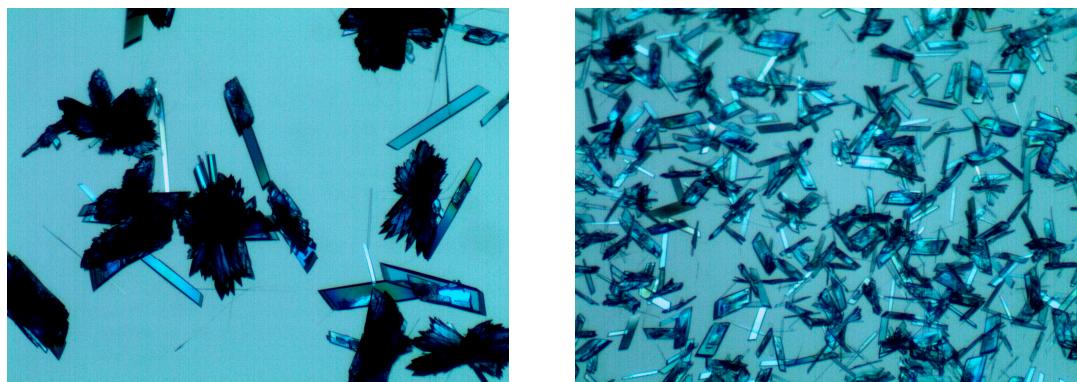
Homa Mousavi, María Eugenia García-Rubiño, Duane Choquesillo-Lazarte, Alfonso Castiñeiras, Luis Lezama, Antonio Frontera and Juan Niclós-Gutiérrez\*

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**Figure S1.** FT-IR spectra of the binary compound  $[\text{Cu}_2(\mu\text{-EGTA})(\text{H}_2\text{O})_2]\cdot 2\text{H}_2\text{O}$  (up) and the new ternary compound **1** (down).



**Figure S2.** Photos of crystals of compound **(1)**.