

Electronic Supplementary Information for:

New coordination polymers based on the triangular $[\text{Cu}_3(\mu_3\text{-OH})(\mu\text{-pz})_3]^{2+}$ unit and unsaturated carboxylates

by

Simone Contaldi, Corrado Di Nicola, Federica Garau, Yauhen Yu. Karabach, Luísa M. D. R. S. Martins, Magda Monari,* Luciano Pandolfo,* Claudio Pettinari,* Armando J. L. Pombeiro*

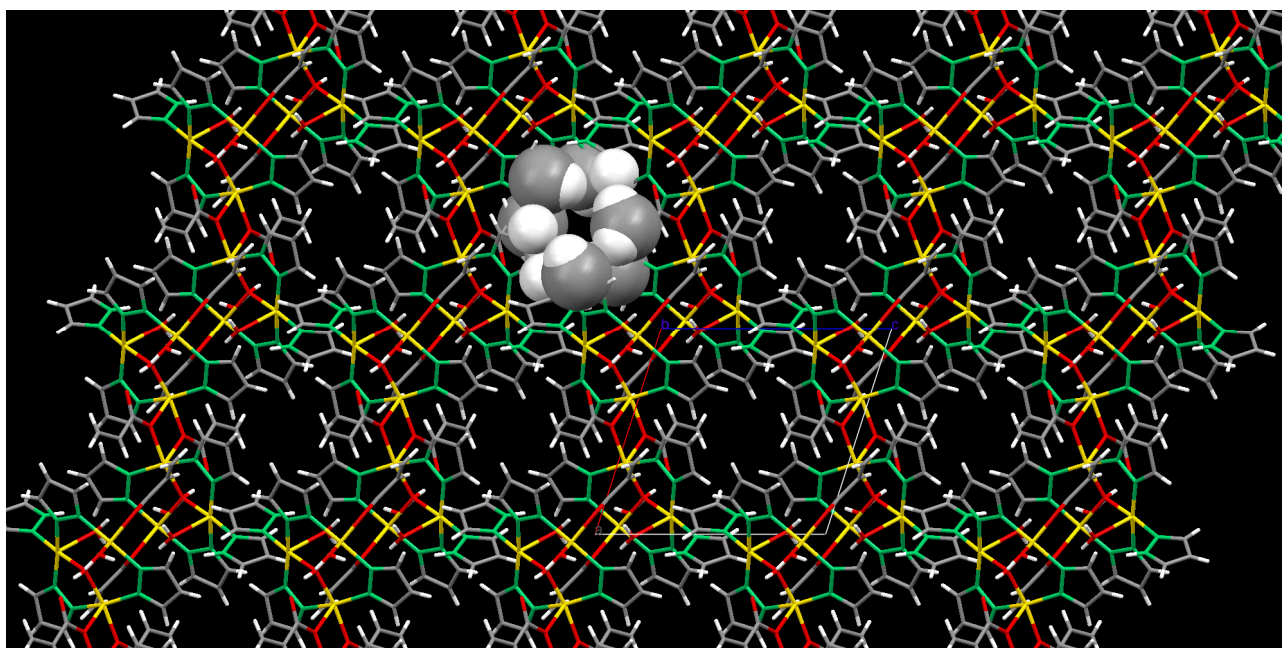


Figure S1 - Capped-stick representation of the crystal packing of **1** with evidenced in space-fill mode the small channels running down *b* crystallographic axis.

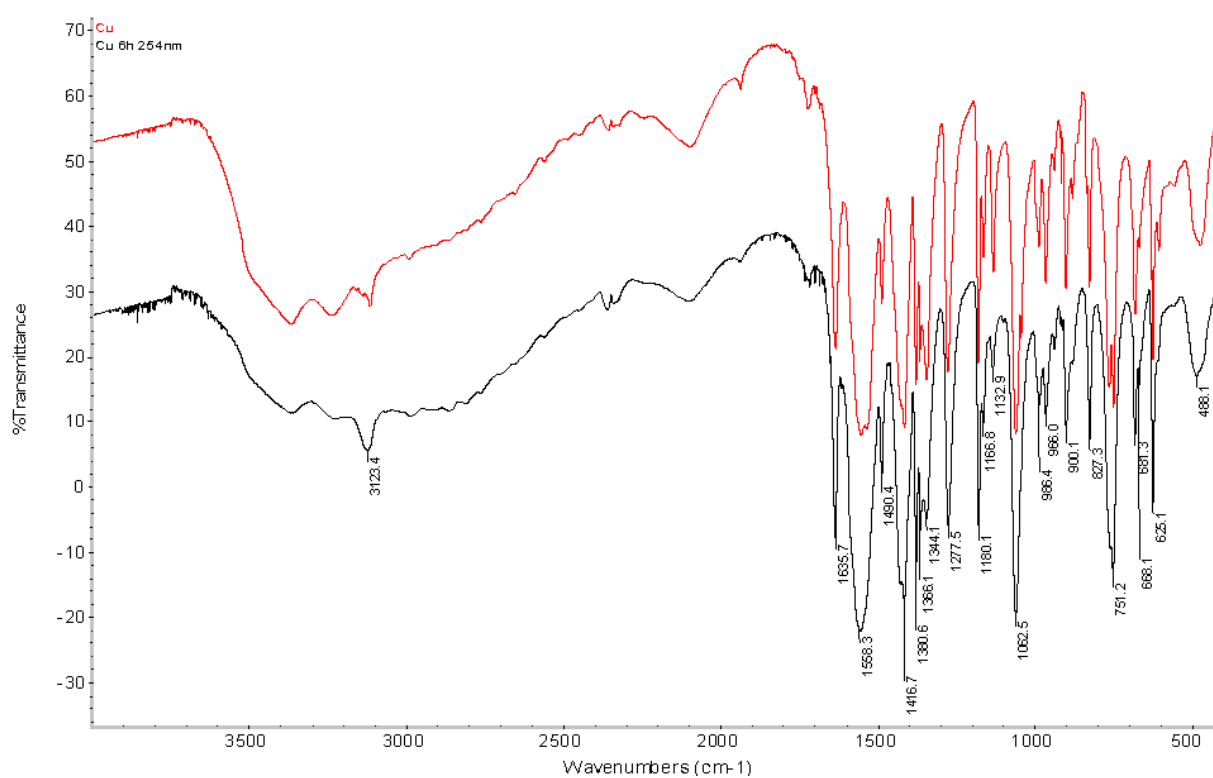


Figure S2 - IR spectra of **1** before (red) and after (black) UV irradiation.

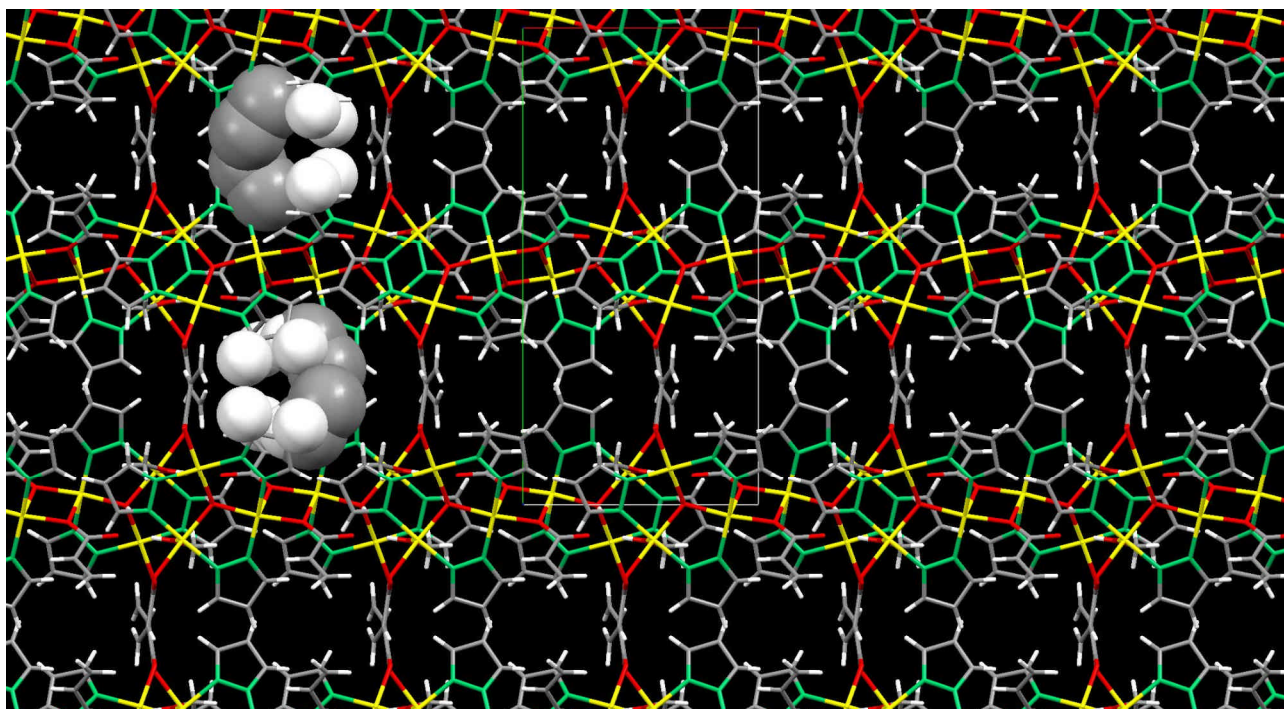


Figure S3 - Capped-stick representation of the crystal packing of **2** with evidenced in space-fill mode the small channels running down *c* crystallographic axis.

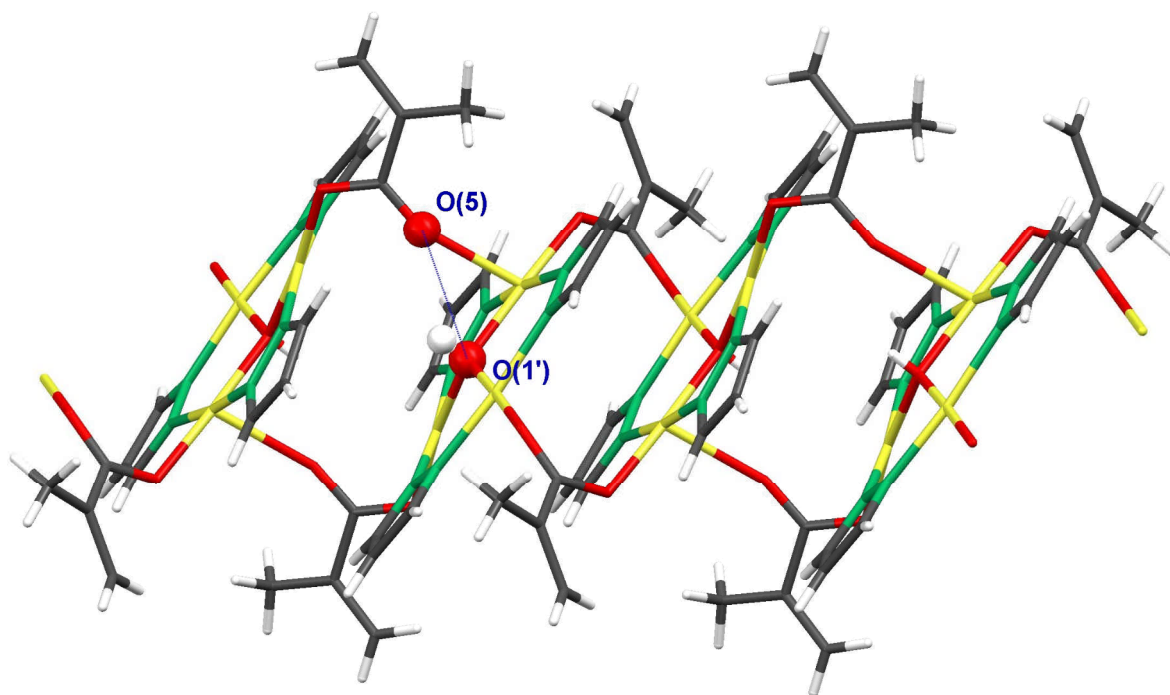


Figure S4 – Representation of one H-bond present in the supramolecular structure of **3**.

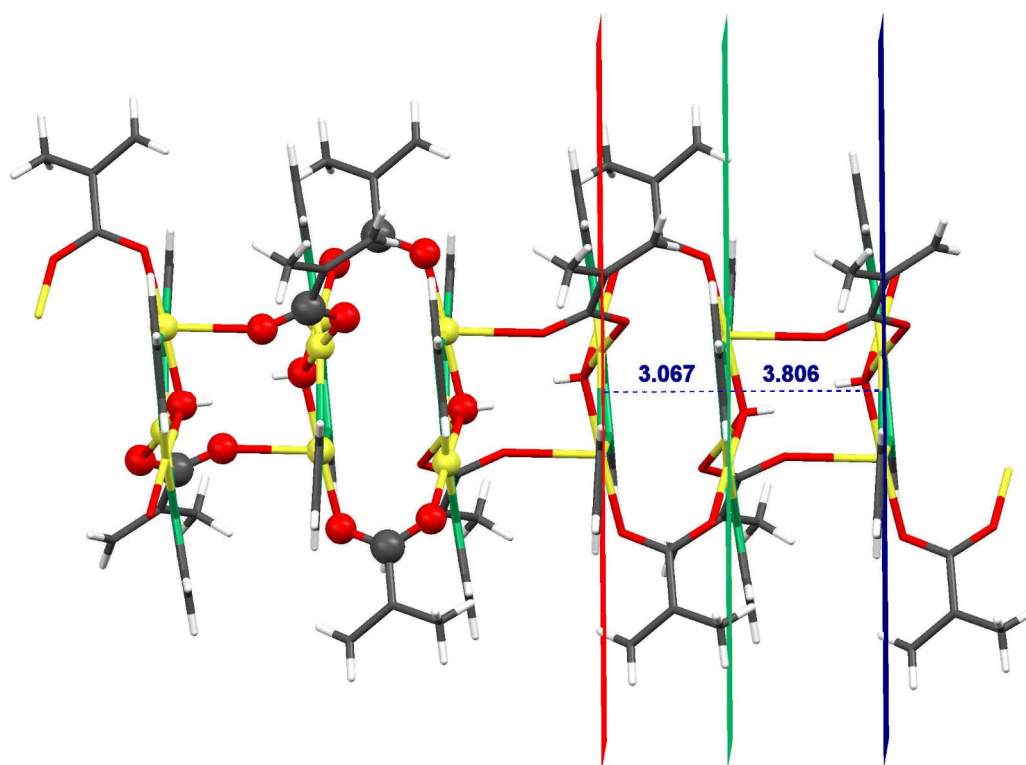
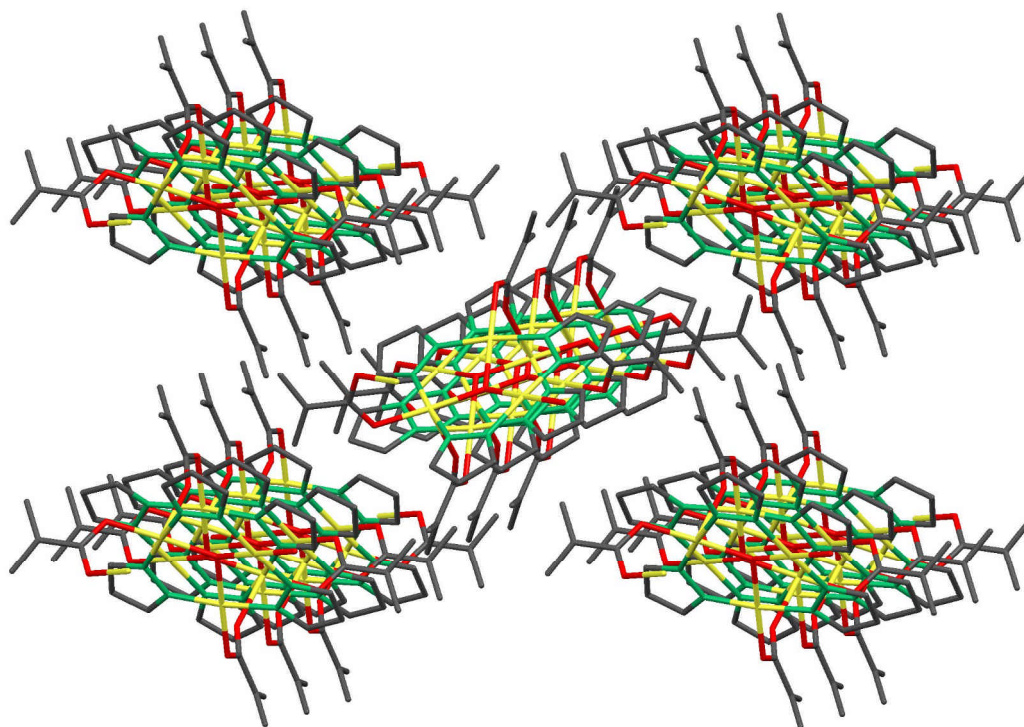
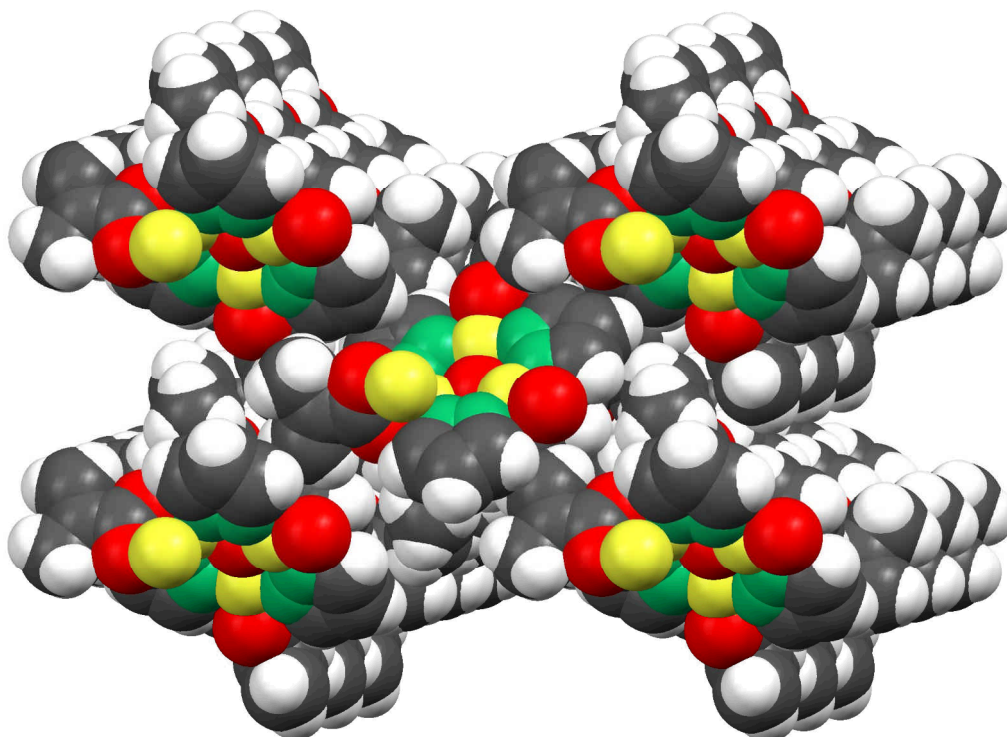


Figure S5 – Capped-stick representation of 1-D MOF of compound **3**. In ball-and-stick are evidenced the couples of *syn-syn* and *syn-anti* carboxylates forming different rings joining trinuclear copper clusters. The distances between the planes defined by Cu(1), Cu(2) and Cu(3) of three adjacent trinuclear triangular clusters (*ca.* 3.067 and 3.806 Å) are also shown.



a



b

Figure S6 – a) Crystal packing of **3** showing five parallel 1-D MOFs running down the crystallographic *a* axis. H atoms have been removed for sake of clarity; b) Space-filling representation evidencing the lack of any pore or channel in **3**.

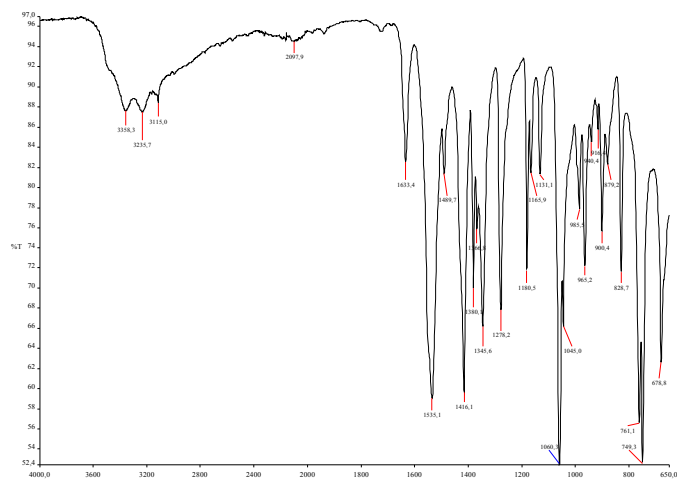


Figure S7 – IR spectrum (KBr) of $[\text{Cu}_3(\text{OH})(\text{C}_3\text{H}_3\text{N}_2)_3(\text{CH}_2=\text{CHCOO})_2(\text{C}_3\text{H}_4\text{N}_2)(\text{H}_2\text{O})_2]$, **1**

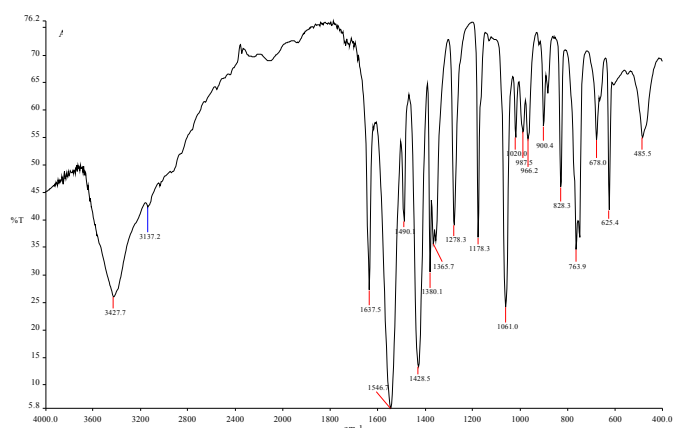


Figure S8 – IR spectrum (KBr) of $[\text{Cu}_3(\text{OH})(\text{C}_3\text{H}_3\text{N}_2)_3(\text{CH}_2=\text{CHCOO})_2(\text{MeOH})]$, **2**

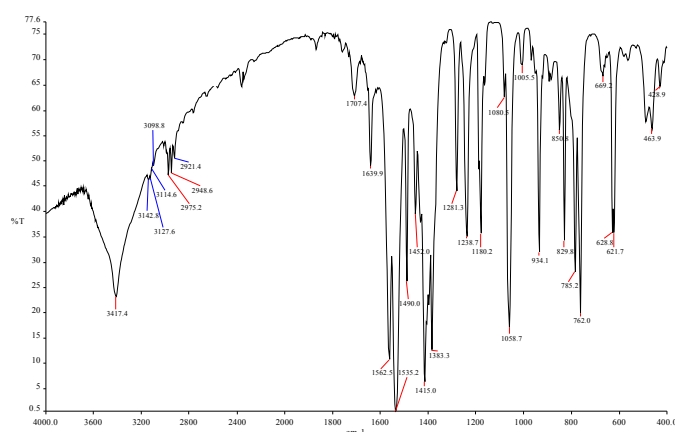


Figure S9 – KBr IR spectrum of $[\text{Cu}_3(\text{OH})(\text{C}_3\text{H}_3\text{N}_2)_3(\text{CH}_2=\text{CHCOO})_2]$, **3**

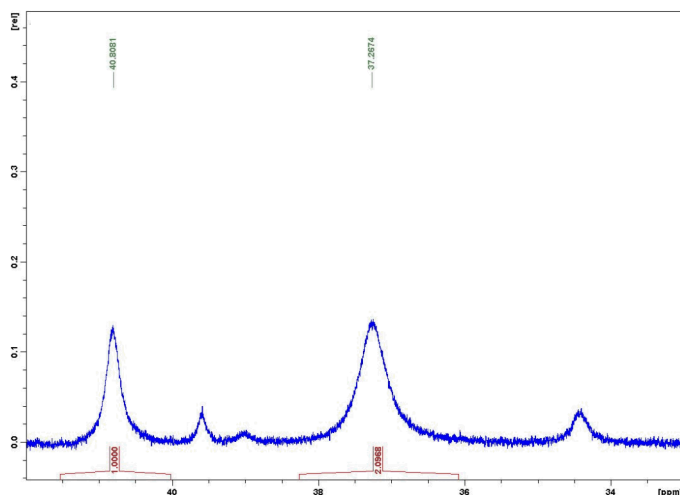


Figure S10 – Low field ^1H NMR spectrum of $[\text{Cu}_3(\text{OH})(\text{C}_3\text{H}_3\text{N}_2)_3(\text{CH}_2=\text{CHCOO})_2(\text{C}_3\text{H}_4\text{N}_2)(\text{H}_2\text{O})_2]$, **1**.

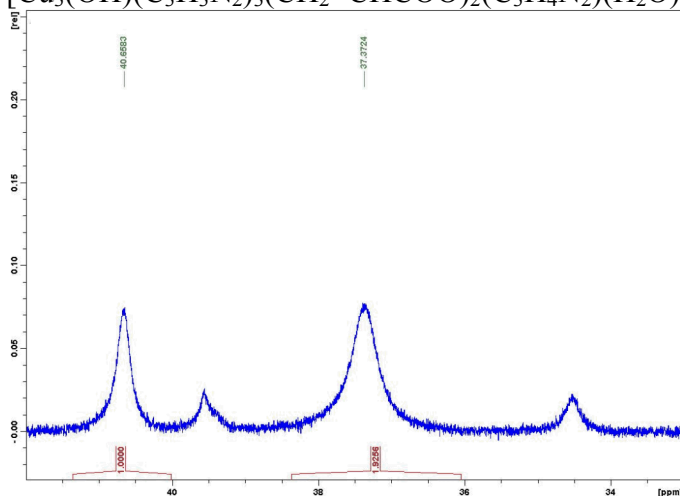


Figure S11 – Low field ^1H NMR spectrum of $[\text{Cu}_3(\text{OH})(\text{C}_3\text{H}_3\text{N}_2)_3(\text{CH}_2=\text{CHCOO})_2(\text{MeOH})]$, **2**.

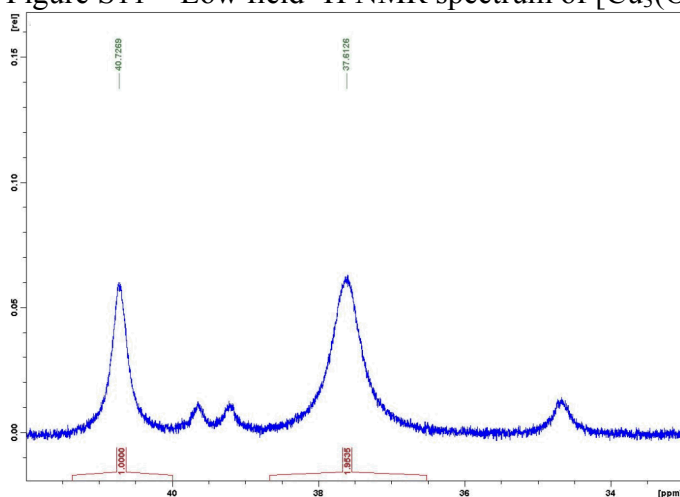


Figure S12 – Low field ^1H NMR spectrum of $[\text{Cu}_3(\text{OH})(\text{C}_3\text{H}_3\text{N}_2)_3(\text{CH}_2=\text{CHCOO})_2]$, **3**

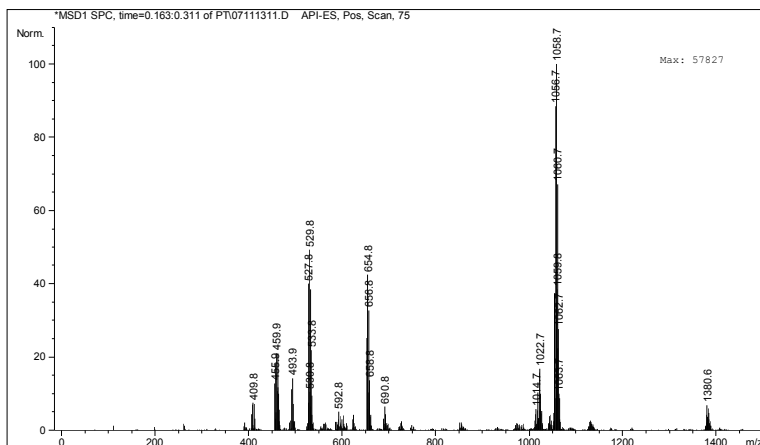


Figure S13 – ESI-MS of $[\text{Cu}_3(\text{OH})(\text{pz})_3(\text{CH}_2=\text{CHCOO})_2(\text{Hpz})(\text{H}_2\text{O})]$, **1**

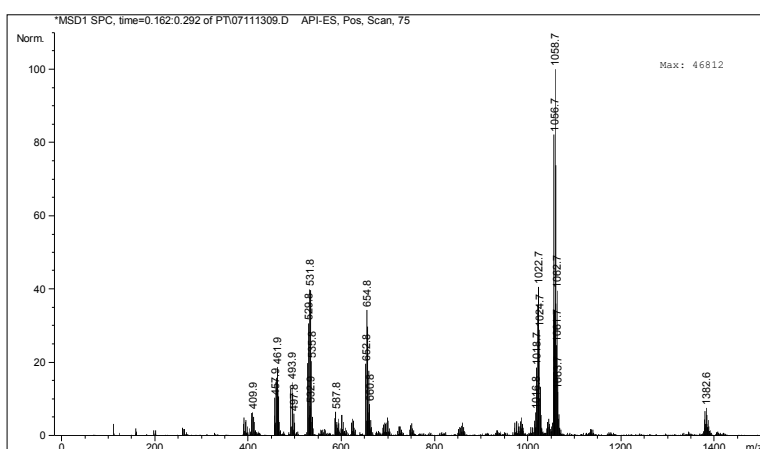


Figure S14 – ESI-MS of $[\text{Cu}_3(\text{OH})(\text{pz})_3(\text{CH}_2=\text{CHCOO})_2(\text{MeOH})]$, **2**

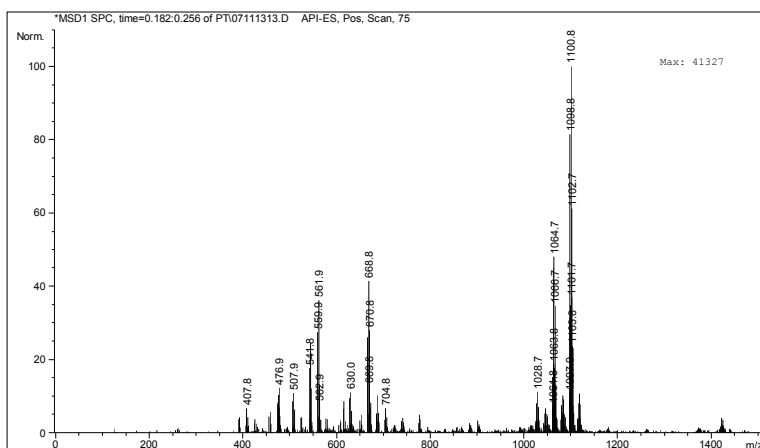


Figure S15 – ESI-MS of $[\text{Cu}_3(\text{OH})(\text{pz})_3(\text{CH}_2=\text{CHCOO})_2]$, **3**