

Supplementary information

of the article

Synthesis, Structural Analysis, and Thermal and Spectroscopic Studies of Methylmalonate-Containing Zinc(II) complexes

Mariadel Déniz,^a Jorge Pasán,^{a,*} Oscar Fabelo,^{a,b} Laura Cañadillas-Delgado,^{a,b,c} Pablo Lorenzo-Luis,^d Fernando Lahoz,^e David López,^e Consuelo Yuste,^f Miguel Julve^f and Catalina Ruiz-Pérez^{a,*}

^aLaboratorio de Rayos X y Materiales Moleculares, Departamento de Física Fundamental II, Facultad de Física, Universidad de La Laguna, Avenida Astrofísico Francisco Sánchez s/n, E-38204 La Laguna (Tenerife), Spain. jpasang@ull.es, caruiz@ull.es

^bInstituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain. / Institut Laue Langevin, 6 rue Jules Horowitz BP 156, 38042 Grenoble, Cedex 9, France.

^cPresent Address: Centro Universitario para la Defensa. Academia General Militar. Ctra de Huesca s/n. 50090 Zaragoza, Spain.

^dDepartamento de Química Inorgánica, Facultad de Química, Universidad de La Laguna, Avenida Astrofísico Francisco Sánchez s/n, E-38204 La Laguna (Tenerife), Spain.

^eDepartamento de Física Fundamental y Experimental, Electrónica y Sistemas, Facultad de Física, Universidad de La Laguna, Avenida Astrofísico Francisco Sánchez s/n, E-38204 La Laguna (Tenerife), Spain

^fDepartament de Química Inorgànica/Institut de Ciència Molecular (ICMol), Facultat de Química, Universitat de València, Polígono La Coma s/n, E-46980-Paterna (València), Spain.

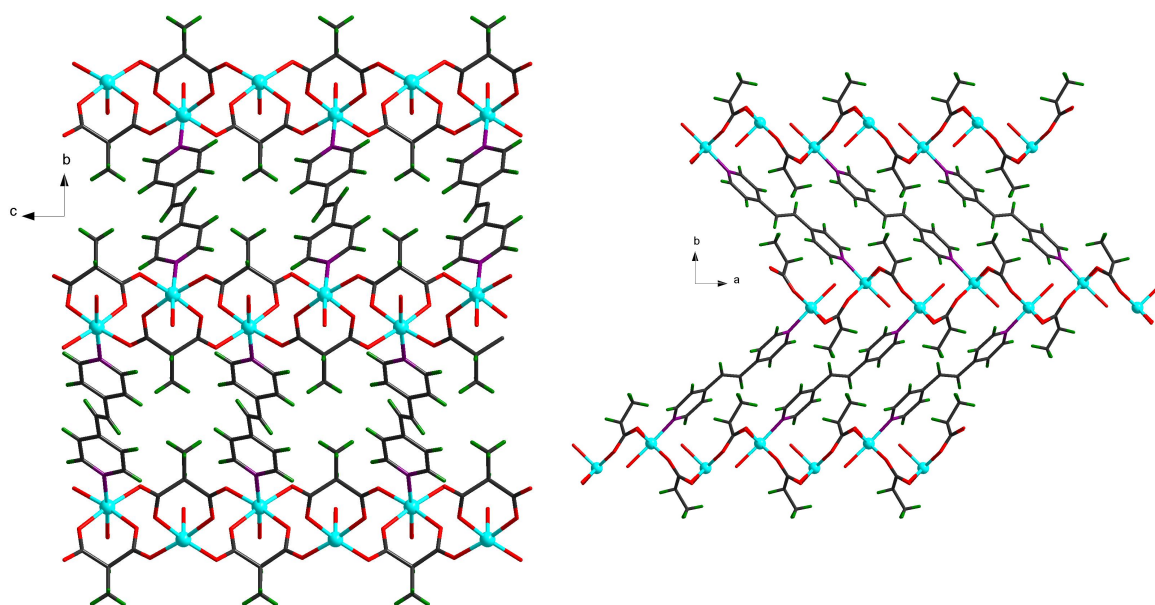


Figure S1. A view of the crystal packing of **3** along the *a* (left) and *c* axes (right).

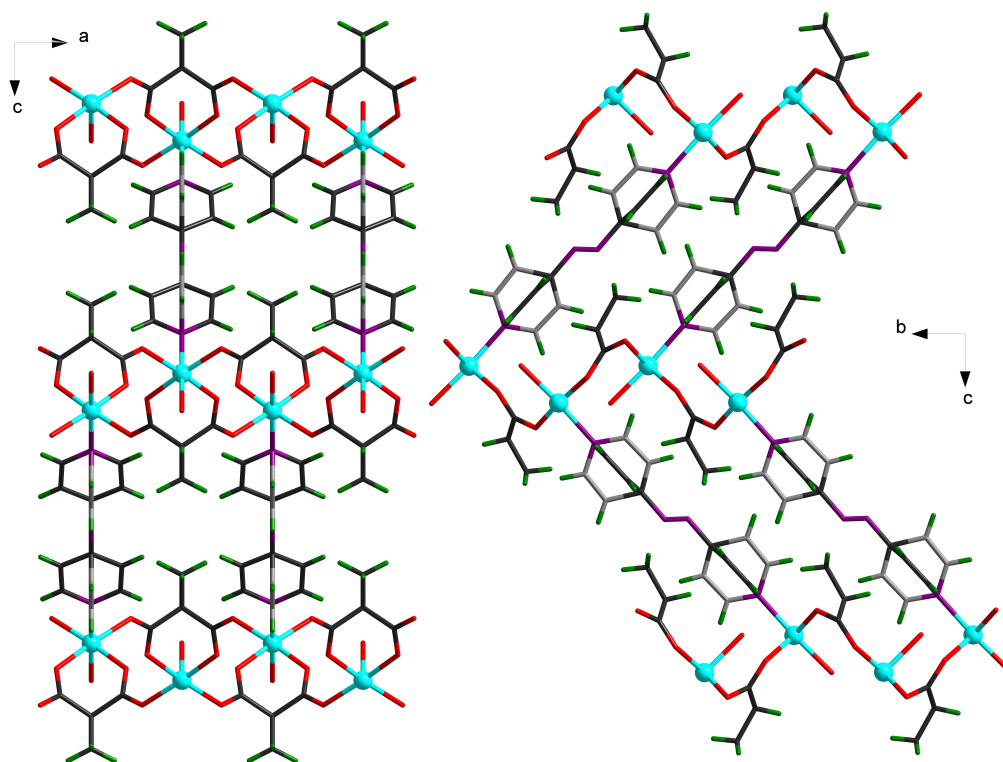


Figure S2. A view of the crystal packing of **5** along the *b* (left) and *a* axes (right). The two possible positions for the pyridyl rings of the azpy ligands have been also depicted.

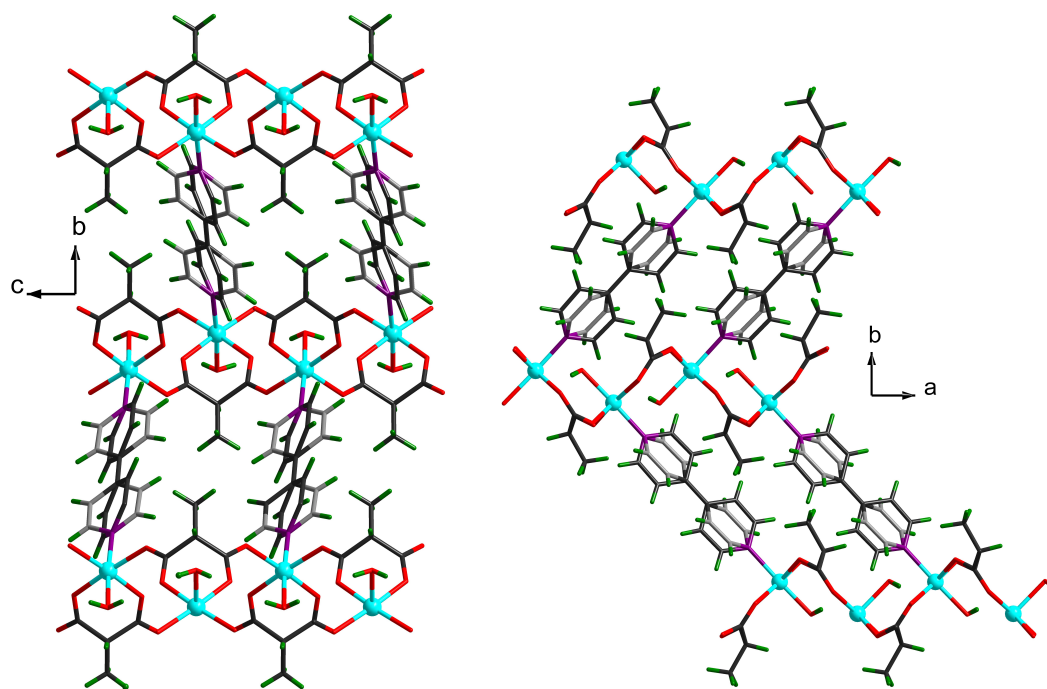


Figure S3. A view of the crystal packing of **2** along the *a* (left) and *c* axes (right). The two possible positions for the pyridyl rings of the 4,4'-bpy ligands have been also depicted.

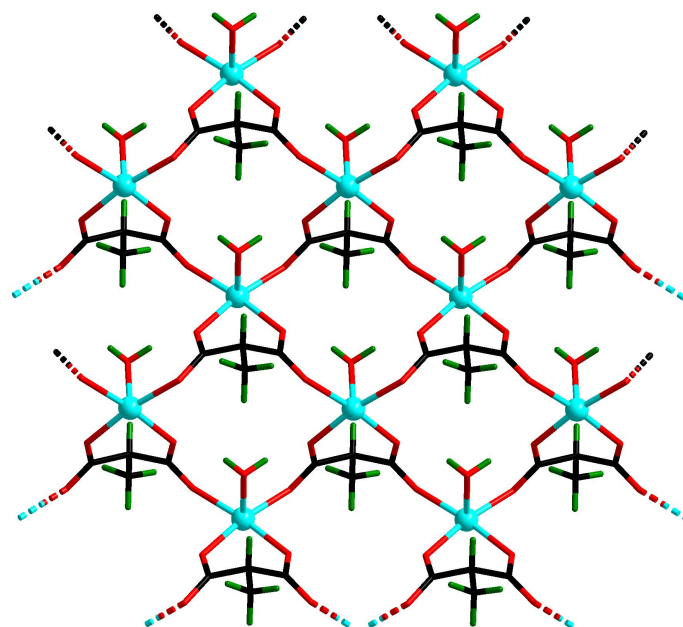


Figure S4. A perspective view of a fragment of the carboxylate-bridged square grid of the zinc atoms in the isostructural compounds **2-5**, which is extended in the *ac* (**2-3**) and *ab* (**4-5**) planes.

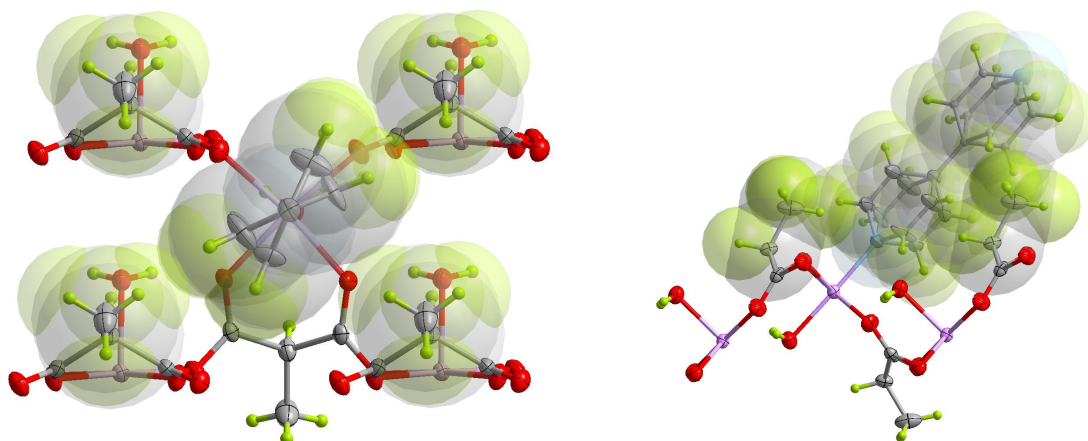


Figure S5. A view of the delocalization of the pyridyl groups of the 4,4'-bpy in **2**. The space filling mode is superimposed to the ortep view to show how the methyl groups preclude the free rotation of the pyridyl, and therefore it has to vibrate around these two main positions.

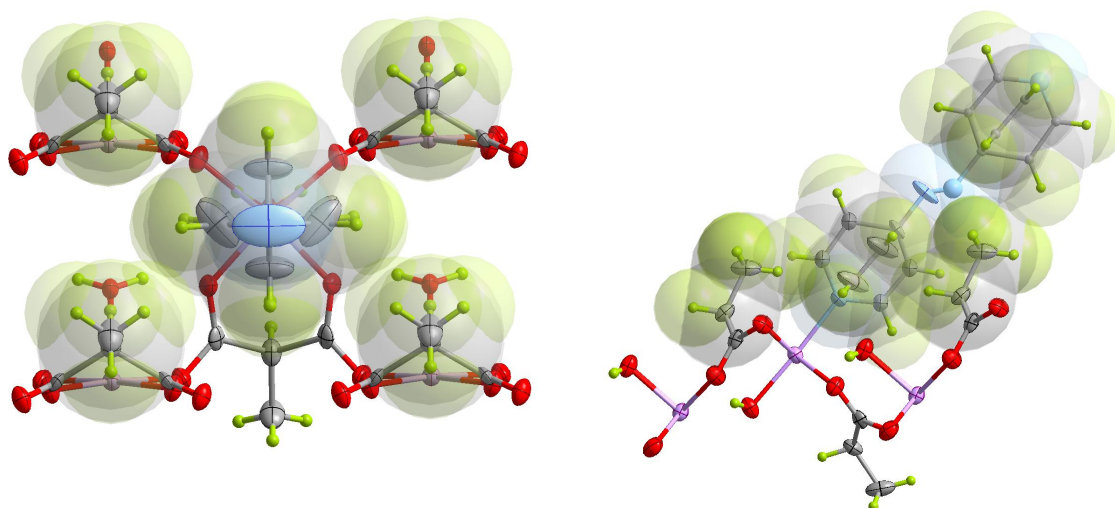


Figure S6. A view of the delocalization of the pyridyl groups of the azpy in **5**. The space filling mode is superimposed to the ortep view to show how the methyl groups allow the free rotation of the pyridyl.

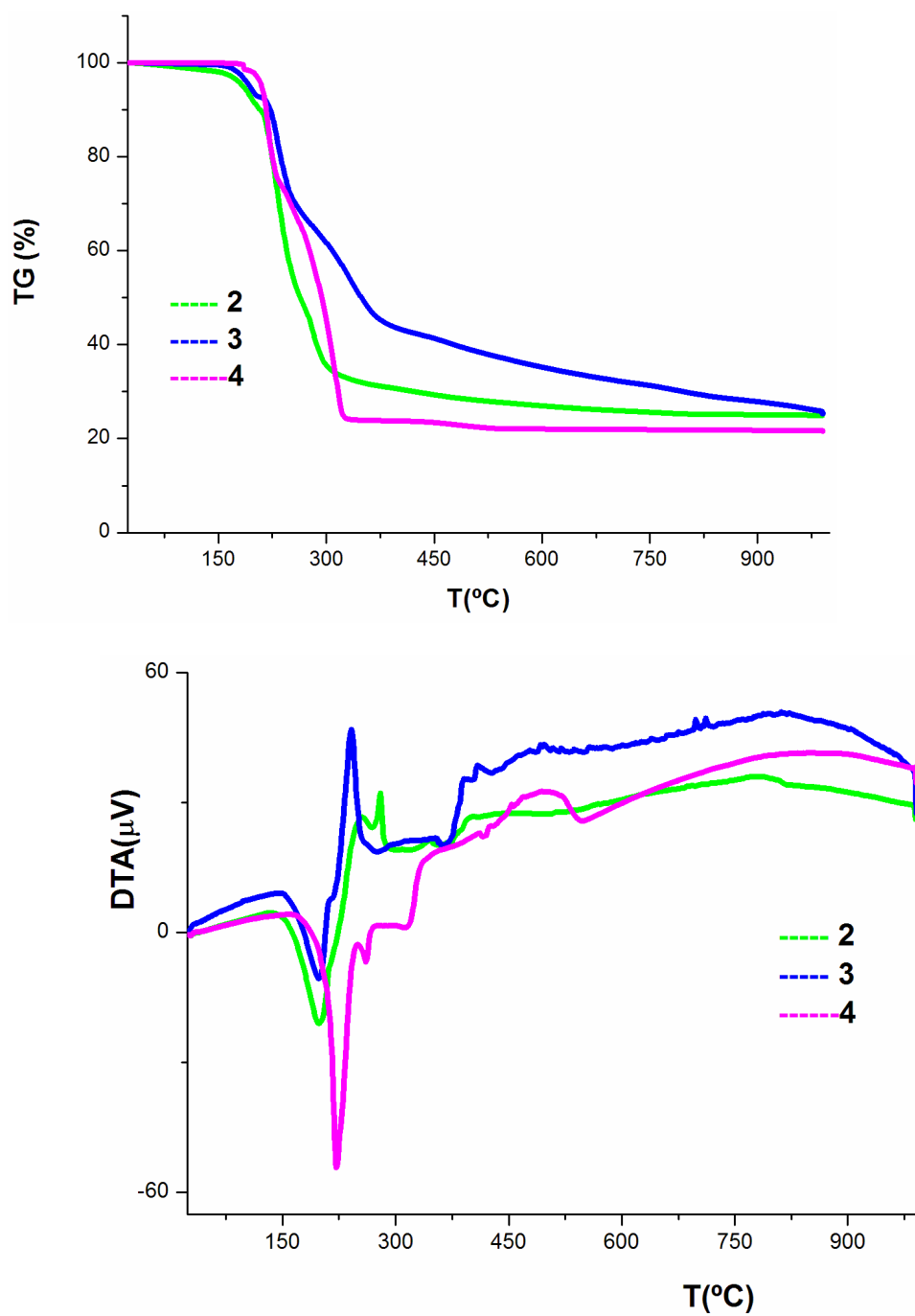


Figure S7. TG/DTG-DTA curves of 2-4 complexes. TG = mass loss (percent); DTA = ΔT (μV) and DTG = percent per minute (\downarrow endo and \uparrow exo).