MS29-1-5 Experimental study of dynamic structural transformations between copper(II) coordination polymers with 5-fluorouracil-1-acetic acid and 4,4-bipyridine
#MS29-1-5

J. Perles [1], P. Amo-Ochoa [1], N. Maldonado [1], A. García [1], V.G. Vegas [1]
[1]Universidad Autónoma de Madrid - Madrid (Spain)

Abstract
The study of chemical systems where slight changes in the synthetic conditions give rise to multiple phases can be very enlightening, especially those where several competing factors are at play (1). In these systems, small variations in solvent ratio, temperature or stoichiometry yield different compounds, which can also undergo phase transformations themselves. These phase transformations, sometimes reversible, as a response to external stimuli (2-3) can be useful to apply these compounds as sensors.
The design of the reported coordination compounds include copper(II) as the metal centre and 4,4-bipyridine and 5-fluorouracil-1-acetic acid (5-FUAcO), a modified nucleobase, as ligands. The use of two ligands with different coordination possiblities allows the formation of compounds with different dimensionality. Furthermore, the interactions of biomolecules with metal ions have proved useful to synthesize biomimetic artificial systems for the development of advanced functional materials that can be applied in therapeutic medicine and materials science (4-5). Biomolecules are also fascinating tools in supramolecular chemistry, as they are well known for their self-recognition ability and stablish a wide variety of non-covalent interactions. Nucleobases in particular have been successfully used as bioligands that can form synthons through supramolecular bonds among themselves, both by hydrogen bonding and π-π stacking interactions, as well as with other molecules (6-8).
In this communication, the different crystal phases (in particular, the six copper coordination polymers obtained), and their transitions are described.

References
1. *Experimental and Theoretical Study of Dynamic Structural Transformations between Sensing Copper(II)-Uracil Antiferromagnetic and Metamagnetic Coordination Compounds.* Maldonado, N.; Perles, J.; Martínez, J. I.; Gómez-García, C. J.; Marcos, M.-L.; Amo-Ochoa, P. Crystal Growth & Des., 2020, 20 (8), 5097-5107.

2. *Smart composite films of nanometric thickness based on copper–iodine coordination polymers. Toward sensors.* Conesa-Egea, J.; Nogal, N.; Martínez, J. I.; Fernández-Moreira, V.; Rodríguez-Mendoza, U. R.; González-Platas, J.; Gómez-García, C. J.; Delgado, S.; Zamora, F.; Amo-Ochoa, P., Chem. Sci. 2018, 9 (41), 8000-8010.

3. *Multistimuli Response Micro- and Nanolayers of a Coordination Polymer Based on Cu_2I_2 Chains Linked by 2-Aminopyrazine.* Conesa-Egea, J.; Gallardo-Martinez, J.; Delgado, S.; Martinez, J. I.; Gonzalez-Platas, J.; Fernandez-Moreira, V.; Rodriguez-Mendoza, U. R.; Ocón, P.; Zamora, F.; Amo-Ochoa, P., Small 2017, 13 (33).

4. *Copper(II)–Thymine Coordination Polymer Nanoribbons as Potential Oligonucleotide Nanocarriers.* Vegas, V. G.; Lorca, R.; Latorre, A.; Hassanein, K.; Gómez-García, C. J.; Castillo, O.; Somoza, Á.; Zamora, F.; Amo-Ochoa, P. Angew. Chem. Int. Ed., 2017, 56 (4), 987-991.

5. *Rational Design of Copper(II)–Uracil Nanoprocessed Coordination Polymers to Improve Their Cytotoxic Activity in Biological Media,* Vegas, V. G.; Latorre, A.; Marcos, M.-L.; Gómez-García, C.J.; Castillo, O.; Zamora, F.; Gómez, J.; Martínez-Costas, J.; Vázquez López, M.; Somoza, A.; Amo-Ochoa, P. ACS Applied Materials & Interfaces, 2021,13 (31), 36948-36957.

6. *Theophylline alkaloid as glue of paddle-wheel copper(II)-adenine entities to afford a rhomboid chain.* Pascual-Colino, J.; Beobide, G.; Castillo, O.; Luque, A.; Pérez-Yáñez, S., Inorg. Chim. Acta, 2019, 484, 437-442.

7. *Reactivity of homoleptic and heteroleptic core paddle wheel Cu(II) compounds.* Sánchez-Férez, F.; Guerrero, M.; Ayllón, J. A.; Calvet, T.; Font-Bardia, M.; Planas, J. G.; Pons, J.,. Inorg. Chim. Acta 2019, 487, 295-306.

8. *Coordination polymers with nucleobases: From structural aspects to potential applications.* Amo-Ochoa, P.; Zamora, F., Coord. Chem. Rev. 2014, 276, 34-58.

Structural diversity in the polymeric compounds