

# Poster Presentations

## [MS24-P34] Synthesis and structural analysis of cadmium-organic dimers, tetramers and polymers – polymorphism and porosity.

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Coordination polymers, infinite systems built up of metal ions and organic ligands have been extensively studied in materials and supramolecular chemistry due their structural diversity and application as porous materials, in catalysis, ion exchange, gas storage and purification. [1] We have investigated the construction of coordination polymers using cadmium as the metal centre and dipicolinic acid, trimesic acid and 1,2-bis(4-pyridyl)ethane as ligands with a view of producing porous materials which may be used for the sorption of gases. The experimental parameters of concentration and time of heating proved to be crucial in the construction of dimers, tetramers and 1D polymers using dipicolinic acid only as the ligand. The 1D polymers yielded an interesting case of polymorphism which was further investigated by density functional theory modeling, this being, to the best of our knowledge, the first combined experimental and theoretical study on the polymorphism of any coordination polymer. A novel, 2-fold interpenetrated, pillared, cadmium metal-organic framework was also synthesized using trimesic acid and 1,2-bis(4pyridyl)ethane. Single crystal X-ray analysis revealed a 2fold interpenetrated, 3-dimensional framework which exhibits a 3,5-connected network with the Schläfli symbol of  $[(6^3)(6^9.8)]$  and *hms* topology. This compound exhibits a temperature-induced single-to-crystal-single-crystal (SC–SC) transformation upon the release of N,N'-dimethylformamide (stable up to 300 °C). SC–SC transformation was also observed when the desolvated form absorbed

selected polar and non-polar organic solvents. In addition, gas (N<sub>2</sub>, CO<sub>2</sub> and N<sub>2</sub>O) sorption experiments were performed showing 2.5% N<sub>2</sub>, 4.5% CO<sub>2</sub> and 3.4% N<sub>2</sub>O absorption by mass at room temperature and moderate gas pressures (~10 bar).

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[2] B. Kukovec, B-M., Venter, G.A., Oliver, C.L., (2012), *Crystal Growth & Design*, **12**, 456-465.

[3] Husain, A., Ellwart, M., Bourne, S.A., Öhrström, L., Oliver, C.L., (2013), *Crystal Growth & Design*, **13**, 1526-1534.

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