22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

Tuning the topology from (4,4)-connected to (6,3)-connected net in Cd (II) coordination polymers: synthesis, crystal structure and Hirshfeld surface analysis

Bahareh Rezaei Kheirkhah, Ghazale Khorshidi and Behrouz Notash*

Department of Inorganic Chemistry, Shahid Beheshti University, 1983969411, Tehran, Iran.

* *E-mail: b_notash@sbu.ac.ir*

Coordination polymers (CPs) defined as coordination compounds with extended bonding in one, two, or three dimensions have become one of the main objects of study in crystal engeenering due to their potential applications in sensing [1], catalyst [2], gas storage and separation [3], drug delivery [4], and so on. The preparation of CPs in which the network topology is controlled by reaction condition is an important step in the design of new functional materials.

In this regard, we report the synthesis of two CPs, namely $[Cd(L)(NO_3)_2(H_2O)]_n$ (**1**) and $\{[Cd(L)_{1.5}(NO_3)_2](MeCN)\}_n$ (**2**), by the self-assembly process using cadmium (II) ion as metal nodes and pyridine containing ligand as linker in MeCN and EtOH/MeCN, respectievly. These compounds were structurally characterized by single-crystal X-ray diffraction analysis and further characterized by powder X-ray diffraction (PXRD). As depicted in Fig. 1, topology of compound **1** can be considered as (4,4)-connected net, while the topology of compound **2** is (6,3)-connected network. Hirshfeld surface analysis of the structures **1** and **2** have been performed and find the percent of participation of intermolecular interactions in the crystal packing of compounds.

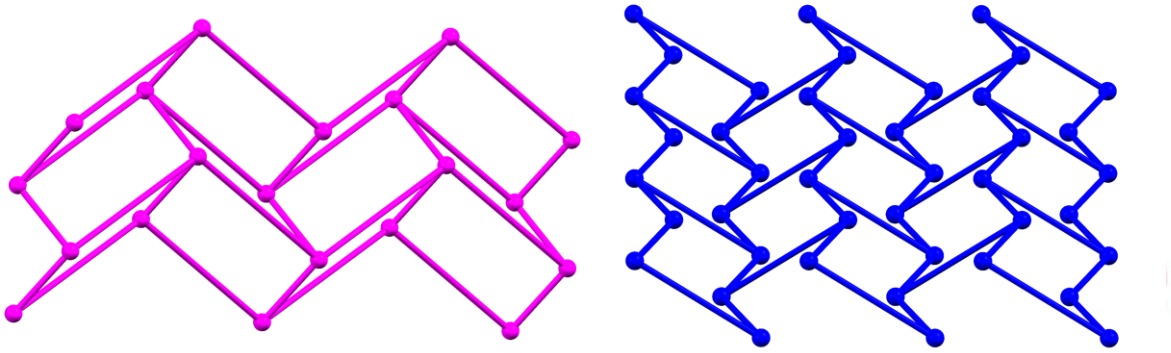


Fig. 1. Schematic view of the (4,4)-connected topology in **1** (left) and (3,6)-connected topology in **2** (right).

Keywords: coordination polymer, cadmium, topology, solvent effect.

References

[1] X. Wang, Y. Wang, N. Xu, J. Ma and G. Liu, *CrystEngComm*, **2023**, 25, 1186.
[2] S. Sahoo and D. Sarma, *Cryst. Growth Des.*, **2022**, 22, 5645.
[3] D. X. Xue, Q. Wang and J. Bai, *Coord. Chem. Rev.*, **2019**, 378, 2.
[4] Z. Zhou, M. Vazquez-Gonzalez and I. Willner, *Chem. Soc. Rev.*, **2021**, 50, 4541.