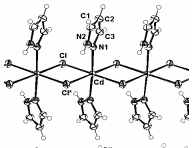
2D Supramolecular Sheet Generated by π Interactions for Cadmium(II) Compounds

Janaina G. Ferreira[1], R. H. A. Santos[1], P. B. da Silva[2], R. C. G. Frem[2], A. V. Godoy Netto[2], A. E. Mauro[2], *[1]Instituto de Química de São Carlos, USP, C.P. 780, 13560-970, São Carlos-S.P., Brazil. [2]Instituto de Química de Araraquara, UNESP, C.P. 355, 14801-970, Araraquara-S.P., Brazil*. E-mail: janagofe@iqsc.usp.br

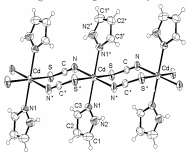
The X-ray structure determinations showed that the coordination polymers $[Cd(\mu\text{-}Cl)_2(HPz)_2]_n$ (**1**) and $[Cd(\mu\text{-}1,3\text{-}SCN)_2(HPz)_2]_n$ (**2**) (HPz = pyrazole) exhibited chain structures made by linear arrays of Cd(II) bridged by chlorine (**1**) (see Fig. 1) or 1,3-SCN (**2**) (see Fig. 2) ions with the pyrazole ligands at the apical sites.

The crystal packing structure of **1** consists of two-dimensional infinite chains along the **b** axis. Hydrogen bonding is the responsible for the self-assembly of linear chains of **1**, yielding a 2D network Intramolecular hydrogen bonds also occur between N-H and Cl.

The X-ray single crystal structure of **2** revealed that the closest chains are arranged side by side to facilitate the N-H···π and C-H···π weak interactions, forming 2D sheets. The 2D sheets are further locked by two weaker π···π interactions from de pyrazole rings. The N atom of the thiocyanate is found to be intramolecular hydrogen bonded to an N-H pyrazole.



(1)



(2)

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