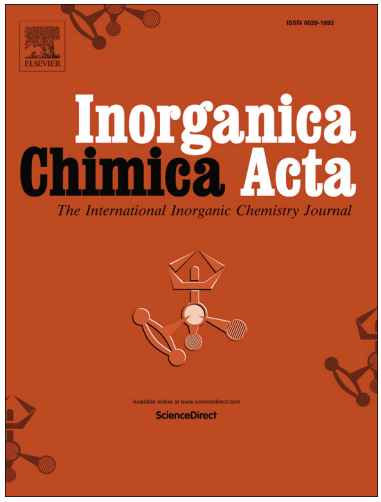

Research paper

Polymeric Ni(II) and Cu(II) complexes based on squaric acid and 1-vinylimidazole: Structural studies and hydrogen adsorption properties

Hakan Yilmaz, Semih Gorduk, Omer Andac

PII: S0020-1693(17)31094-0
DOI: http://dx.doi.org/10.1016/j.ica.2017.09.026
Reference: ICA 17882

To appear in: *Inorganica Chimica Acta*

Received Date: 13 July 2017
Revised Date: 5 September 2017
Accepted Date: 10 September 2017

Please cite this article as: H. Yilmaz, S. Gorduk, O. Andac, Polymeric Ni(II) and Cu(II) complexes based on squaric acid and 1-vinylimidazole: Structural studies and hydrogen adsorption properties, *Inorganica Chimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.ica.2017.09.026

Polymeric Ni(II) and Cu(II) complexes based on squaric acid and 1-vinylimidazole: Structural studies and hydrogen adsorption properties

Hakan Yilmaz [a,*], Semih Gorduk [b,*], Omer Andac [a]

[a] *Ondokuz Mayis University, Faculty of Arts and Sciences, Department of Chemistry, 55139 Samsun, Turkey*

[b] *Yildiz Technical University, Faculty of Arts and Sciences, Department of Chemistry, 34210 Istanbul, Turkey*

Abstract: $[M(sq)(vim)_2(H_2O)_2]_n$ (M: Ni^{2+} and Cu^{2+} ions; sq: squarate dianion; vim: 1-vinylimidazole) complexes were crystallized, and characterized by elemental analysis, infrared spectroscopy (IR), thermal analysis, magnetic susceptibility, powder X-ray diffraction (PXRD) and X-ray single crystal techniques. The results of X-ray single crystal analysis demonstrate that both complexes crystallize in the monoclinic system with $P2_1/n$ space group and have slightly distorted octahedral geometries. In the complexes, the sq ligand behaves as bis(monodentate) via the oxygen atoms in trans-(μ-O^1,O^3) mode and the vim ligand coordinates to the metal ions via the ring nitrogen atom as monodentate. The complexes have one-dimensional (1D) polymeric chains constructed from the connecting of metal ions to each other by the sq ligands. The linking of 1D polymeric chains with the hydrogen bonds leads to the formation of two-dimensional (2D) supramolecular structures. The π-π interactions also contribute to the formation of three-dimensional (3D) supramolecular structures. The surface areas and hydrogen adsorption properties of the complexes were investigated. The accessible surface areas and free volumes of the complexes were also determined by theoretical calculations in 0.8 Å Connolly diameter.

Keywords: Squarate dianion, 1-vinylimidazole, polymeric complex, crystal structure, hydrogen adsorption

[*] Corresponding Authors: Semih Gorduk and Hakan Yilmaz

E-mail: sgorduk@yildiz.edu.tr, Tel: +90 212 383 4131

E-mail: hakan.yilmaz@omu.edu.tr, Tel: +90 362 312 1919