

Title: Synthesis, structure and electrochemical behaviour of Na, Mg-II, Mn-II, Cd-II and Ni-II complexes of 3-(2-carboxyphenylhydrazone)pentane-2,4-dione

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Abstract: Mononuclear manganese(II) [Mn(kappa O-HL)(2)(CH3OH)(4)] (4), nickel(II) [Ni(kappa O-2, kappa N-L)(H2O)(3)] (5), cadmium(II) [Cd(kappa O-2-HL)(2)(CH3OH)(3)] (7), tetranuclear zinc(II) [Zn-4(mu-OH)(2)(1 kappa O:2 kappa O-HL)(4)(kappa O-HL)(2)(H2O)(4)] (6) and polynuclear aqua sodium(I) [Na(H2O)(2)(mu-H2O)(2)](n)(HL)(n) (2) and magnesium(II) [Mg(OH)(H2O)(mu-H2O)(2)](n)(-HL)(n) (3) complexes were synthesized using 3-(2-carboxyphenyl-hydrazone)pentane-2,4-dione (H2L, 1) as a ligand precursor. The complexes were characterized by single crystal X-ray diffraction, elemental analysis, IR, H-1 and C-13 NMR (for 2, 3, 6 and 7) spectroscopies. Mono- or dianionic deprotonated derivatives of H2L display different coordination modes and lead to topologies and nuclearities of the complexes depending on metal ions and conditions used for the syntheses. Extensive intermolecular H-bonds form supramolecular arrangements in 1D chains (4 and 6), 1D chains of the organic anion and 2D networks of the metal-aqua aggregates (2 and 3), 2D networks (7) or even 3D frameworks (5). Electrochemical studies, by cyclic voltammetry and controlled potential electrolysis, show ligand centred redox processes as corroborated by theoretical DFT calculations in terms of LUMO and HOMO compositions. (C) 2012 Elsevier Ltd. All rights reserved.

Author Keywords: Arylhydrazones of beta-diketones; Metal complexes; Structure modulation; DFT calculations

KeyWords Plus: Crystal-Structures; Molecular Machines; Copper(II); NICKEL(II); Ligand; Zinc(II); Density

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