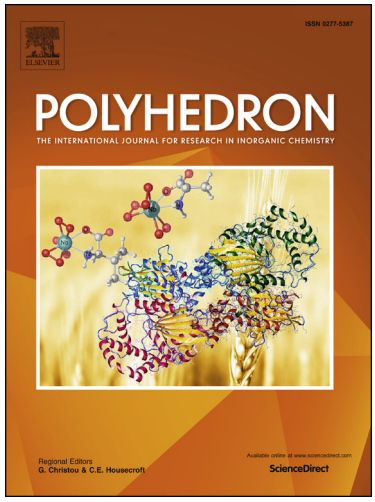

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Synthesis, characterisation and antibacterial activity evaluation of trinuclear Ni(II) complexes with N-substituted salicylhydrazide ligands

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ABSTRACT

Three novel trinuclear Ni(II) complexes, $[Ni_3(L^1)_2(py)_4]$ (**1**), $[Ni_3(L^2)_2(H_2O)_2(DMA)_2]$ (**2**) and $[Ni_3(L^3)_2(py)_4]$ (**3**), with trianionic pentadentate ligands derived from salicylhydrazide with N-acyl substituents [H_3L^1 =N^2-crotonoylsalicylhydrazide, H_3L^2 = N^2-(3,3-dimethylacryloyl)salicylhydrazide, H_3L^3 =N^2-cinnamoylsalicylhydrazide] were synthesized and characterized by elemental analysis, spectroscopic techniques, like UV-Vis, FT-IR and NMR, molar conductivity and magnetic susceptibility measurements, and single crystal X-ray diffraction. The solid state structures of the complexes reveal the binding modes of the different ligands via ONO donor atoms. Complex **1** crystallises in the triclinic system while complexes **2** and **3** crystallise in the monoclinic system with space groups $P\bar{1}$ (**1**) and $P2_1/c$ (**2** and **3**). Computational studies were performed using Density Functional Theory (DFT) to obtain physical properties of all three complexes. The ligands and their metal complexes were screened for antibacterial activity to assess their inhibition potential against two Gram positive bacteria; *S. aureus* and *B. subtilis* and two Gram negative bacteria; *E. coli* and *P. aeruginosa* by the well diffusion method using gentamicin as a positive control. Antibacterial screening data reveals that the trinuclear Ni(II) complexes have significantly enhanced inhibitory activities compared to the ligands.

Keywords

Ni(II) complex, Antimicrobial activity, Salicylhydrazide, Crystal structure, DFT studies

Abbreviations

DMF = *N*,*N*-dimethylformamide, DMA = *N*,*N*-dimethylamine, py = pyridine, DMSO = dimethylsulfoxide, MeOH = methanol, ESI = Electrospray ionisation, SC-XRD = Single crystal X-ray diffraction, HOMO = highest occupied molecular orbital, LUMO = lowest unoccupied molecular orbital

1. Introduction