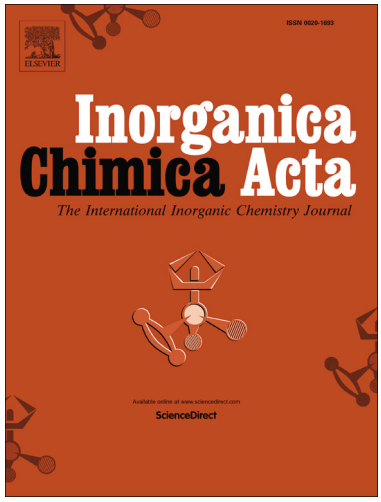

Research paper

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Accurate DFT studies on crystalline network formation of a new Co(II) complex bearing 8−aminoquinoline

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ABSTRACT

As a continuation of our studies on the coordination chemistry of 8−aminoquinoline (8-aq) and related nitrogen-containing heterocyclic ligands, we report the synthesis and crystal structure of a new complex of formula *cis*−[$Co(8-aq)_2(NCS)_2$] (**1**) by slow evaporation of an aqueous ethanolic solution containing a mixture of 8-aq, KSCN, and $Co(NO_3)_2{\cdot}6H_2O$. As expected, the 8-aq ligand chelates to the metal with the resulting coordination sphere being distorted octahedron. Examination of the packing of **1** in the crystal together with the results of high level DFT−D/B3LYP calculations indicate the packing is stabilized by non−classical intermolecular N–H···S, N–H···C, C–H···N, and C–H···S hydrogen bonds (HBs) together with π−stacking interactions. It should be noted that dispersion corrected density functional theory (DFT−D) calculations of the binding energy of non−covalent interactions prove that N–H···S HBs govern the formation of the crystalline 3D network.

Keywords: *cis*−[$Co(8-aq)_2(NCS)_2$]; 8−Aminoquinoline; DFT–D; Non−covalent interaction; Binding energy.