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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)<sub>2</sub>(NCS)<sub>2</sub>] (**1**) by slow evaporation of an aqueous ethanolic solution containing a mixture of 8-aq, KSCN, and Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O. 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  $\pi$ -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)<sub>2</sub>(NCS)<sub>2</sub>]; 8-Aminoquinoline; DFT-D; Non-covalent interaction; Binding energy.

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