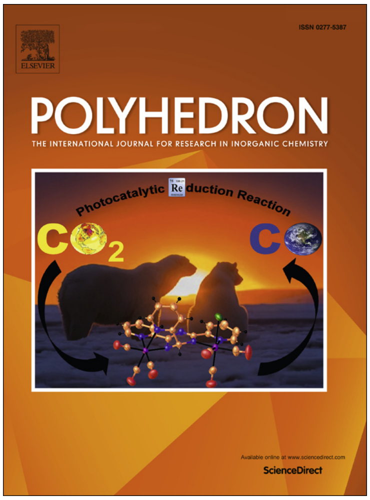

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The role of non-covalent interaction in the hexadentate coordination environment on the magnetic behavior of binuclear helical complex $[Ni2(L)2]^{4+}$: A broken-symmetry approach

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Abstract

The nature of bonds in coordination environments of a homobimetallic supramolecular helicate complex has been studied using Quantum Theory of Atom in Molecule (QTAIM) and the electron localization function (ELF) analysis. The topological parameters at critical points (CPs) indicate that all bonds between nickel ions and ligand donors have non-covalent nature. The lack of any disynaptic basins in coordination environments confirms the QTAIM results. The broken-symmetry (BS) approach has been employed to predict properties of the complex using B3LYP functional and different basis sets for metal ions. The calculated magnetic exchange coupling constants (*J*) are 2683.34 and 2897cm^{-1} for different metal basis sets. The NBO analysis has been performed to explain the role of coordination bonds nature in strong ferromagnetic behavior of the complex.

Keywords: Ferromagnetic behavior; Broken-symmetry; Non-covalent interaction; DFT.

1. Introduction

Despite there are several studies on the effect of the magnetic centers coupler properties on magnetic behavior of the systems [1-11], the nature of bonds between spin centers and the couplers is less paid attention.

The enhancing of the magnetic exchange coupling constants by increasing conjugation and aromaticity degrees of couplers are two common strategies to design stronger molecular magnets [4-11]. Transition metal ions may act as spin centers. Many experimental efforts have been made to improve the magnetic properties of transition metal complexes by bridging ligand modification to facilitate magnetic interactions between transition metal ions [12-18]. However,