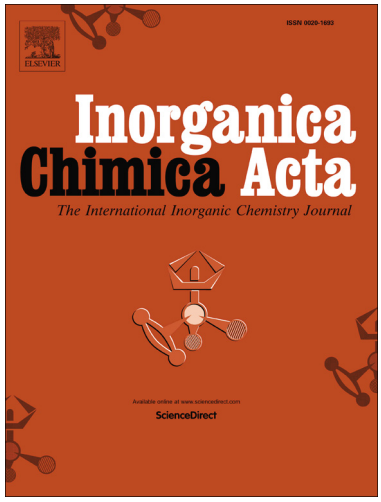

Research paper

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Strong metallophilic interactions in nickel coordination compounds

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Abstract

The upper limit for energy of strongest and extremely short metallophilic interactions Ni•••Ni in nickel coordination compounds and their supramolecular associates obtained from the Cambridge Structural Database has been estimated by using DFT calculations followed by the topological analysis of the electron density distribution within the framework of Bader's theory (QTAIM method) in accordance with Espinosa's or Vener's approaches. The covalent contribution in all discussed ligand-supported contacts Ni•••Ni is significant, whereas majority of ligand-unsupported metallophilic interactions Ni•••Ni have purely non-covalent nature. The upper limit for energy of studied strong metallophilic interactions in nickel coordination compounds is 23 and 6 kcal/mol (ligand-supported and ligand-unsupported cases, respectively). All studied ligand-supported and ligand-unsupported metallophilic interactions Ni•••Ni have attractive nature.

Keywords

nickel, non-covalent interactions, metallophilic interactions, DFT, QTAIM