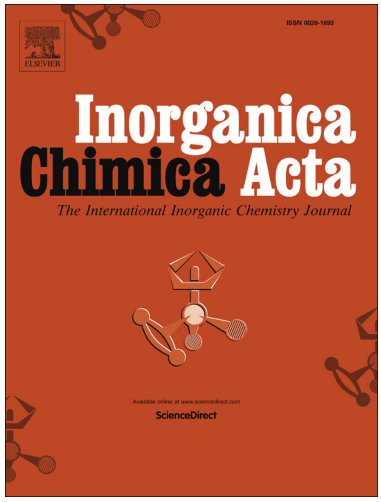

Research paper

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Theoretical confirmation of existence of X•••Au non-covalent contacts

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Abstract

The supramolecular assembly based on various intermolecular interactions involving metal centers currently is cutting edge topic in coordination chemistry community. Meanwhile, there are several reports whose authors simply did not pay any attention to the phenomenon of metal-involving X•••Au (X = I, Cl) non-covalent contacts. We have proved the existence of such non-covalent interactions in model structures for the solvates $[Au(CN)_2]^-•CH_2Cl_2$ and $[AuBr_2]^-•(C_2I_4)_4$ using DFT calculations followed by the topological analysis of the electron density distribution within the formalism of Bader's theory (QTAIM method) based on the experimental geometrical parameters. The appropriate bond critical points (3, –1) were located and energies for these weak contacts (2–5 kcal/mol) were estimated.

Keywords

Non-covalent interactions, DFT calculations, QTAIM

1. Introduction

Non-covalent interactions involving halogen atoms is a paradigm [1] and a cutting edge topic in the modern supramolecular chemistry [2], crystal (in particular, liquid crystal [3]) engineering [4, 5], nonlinear optics [6, 7], drug design [8, 9], and polymers science [10]. These non-covalent