

Poster Presentation

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Supramolecular organization of complexes of aryl hydrazones with SnCl₃ and SnCl₄

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Chelate complexes of main group metals with N,O-chelating Schiff Base ligands have been reported as perspective models for biologically active species. The derivatives of aryl hydrazones are among the most widely used ligands of such type. In our study, crystal structures of aryl hydrazones with SnCl₃ and SnCl₄ are discussed: the presence of aromatic fragments, amine groups and chlorine atoms therein are responsible for the coexistence of strong hydrogen and halogen bonds as well as stacking and Cl... π interactions. Interplay between these types of interactions and their role in stabilization of crystal structures is the subject of particular interest. We studied all these aspects in complexes of aryl hydrazones using different theoretical approaches: those based on Stockholder partitioning, molecular electrostatic potential, non-covalent interaction index, AIM theory – together with Espinosa-Mollins-Lecomte correlation to estimate the energy of all intermolecular interactions in crystals by means of electron density analysis from periodic quantum chemical calculations (VASP code). Our results showed that the presence of intermolecular interactions led to a noticeable redistribution of electron density in crystal as compared to an isolated molecule. Although Cl... π , stacking interactions and halogen bonds are numerous in the crystals of these complexes, their contribution to the energy of their crystal lattice does not exceed 30%. The work was supported by Council of the President of the Russian Federation (grant MD-3589.2014.3).

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