

The study of intermolecular complexes of dimethylselenide with ν -acceptors: quantum-chemical aspects

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Keywords: organoselenium compounds, intermolecular complexes, ν -acceptors, Quantum theory of Atoms in Molecules, Interacting quantum atom approach, nature of intermolecular interactions.

Abstract

Complexes of dimethylselenide with some ν -acceptors of different strength were studied by density functional theory approach (B3LYP/6-311++G(d,p)). The sharing of electron density was found to play more important role in comparison with electrostatic interaction between components of the complex. Topological analysis of the electron density revealed that the nature of the intermolecular bond varies from van der Waals to weak covalent. The role of electrostatic and exchange-correlation contribution to $Se...Al$ interaction and intermolecular bonding was studied on the example of $H_2Se...AlH_3$ complex by means of interacting quantum atom approach.