

## The nature of the interaction of dimethylselenide with IIIA group element compounds

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### Abstract

The first systematic theoretical study of the nature of intermolecular bonding of dimethylselenide as donor and IIIA group element halides as acceptors was made with the help of the approach of Quantum Theory of Atoms in Molecules. Density Functional Theory with "old" Sapporo triple- $\zeta$  basis sets was used to calculate geometry, thermodynamics, and wave function of Me<sub>2</sub>Se $\cdots$ AX<sub>3</sub> complexes. The analysis of the electron density distribution and the Laplacian of the electron density allowed us to reveal and explain the tendencies in the influence of the central atom (A = B, Al, Ga, In) and halogen (X = F, Cl, Br, I) on the nature of Se $\cdots$ A bonding. Significant changes in properties of the selenium lone pair upon complexation were described by means of the analysis of the Laplacian of the charge density. Charge transfer characteristics and the contributions to it from electron localization and delocalization were analyzed in terms of localization and delocalization indexes. Common features of the complexation and differences in the nature of bonding were revealed. Performed analysis evidenced that gallium and indium halide complexes can be attributed to charge transfer-driven complexes; aluminum halides complexes seem to be mainly of an electrostatic nature. The nature of bonding in different boron halides essentially varies; these complexes are stabilized mainly by covalent Se $\cdots$ B interaction. In all the complexes under study covalence of the Se $\cdots$ A interaction is rather high. © 2013 American Chemical Society.

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