Russian Chemical Bulletin 2014 vol.63 N1, pages 43-53

Dimethyl selenide complexes with compounds of Group IIIA elements: Electron density redistribution and interaction energy partitioning

Madzhidov T., Chmutova G.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Molecular structures of dimethyl selenide complexes with AX3 (A = B, Al, Ga, In; X = H, Me) compounds of Group IIIA elements were calculated by the PBE1PBE/SapporoTZ method. A complex approach to study the nature of interactions is proposed, which involves analysis of electron localization/delocalization characteristics and their influence on charge transfer and energy effects of complexation. It is shown that electron sharing is more important for stabiliza tion of the complexes under study than electrostatic interaction between their fragments. It is demonstrated that analysis of local (topological) characteristics of the electron density distribu tion is insufficient to discover similarity/dissimilarity in the nature of some complexes. The energies of interaction in the complexes under study are mainly composed of the contributions of Se atom as active center of the donor molecule and the entire acceptor molecule. Energy characteristics of local interaction between Se atom and Group IIIA element atom are not representative.

http://dx.doi.org/10.1007/s11172-014-0392-2

Keywords

Density functional theory, Interacting quantum atoms (IQA) approach, Intermolecular complexes, Nature of intermolecular inter actions, Organoselenium compounds, PBE1PBE functional, Theory of atoms in molecules (AIM)