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Theoretical Study of σ-hole Bonding between Selenium Atoms in Crystal Structures of Organoselenium Compounds

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Non-covalent interactions involving selenium atoms are of great importance in chemistry and biochemistry due to the prominent role of selenium-containing molecules (like Se-antioxidants and selenoenzymes) in different biochemical processes. [1] Although studies of non-covalent interactions of chalchogen atoms are mainly focused on their role in hydrogen bonding, in the last decades another type of contacts based on σ-hole interactions was recognized as an important factor in non-covalent bonding of these elements. [2] Energetic characteristic and the nature of chalchogen interaction are mainly investigated by quantum chemical calculations, especially in the case of interactions involving sulfur atoms. [3] However, there are no systematic studies related to the nature of selenium-selenium interactions. In this work, we combined analysis of crystallographic data extracted from crystal structures of selenium-containing molecules with the quantum chemical calculations to reveal the energy and geometry of selenium-selenium interactions in crystal structures of organoselenium compounds. In addition, Energy Decomposition Analysis was performed on model systems to reveal the nature of selenium-selenium interactions. Results of analysis of crystal structures were in excelent agreement with the results of quantum chemical calculations performed on model systems. Results of Energy Decomposition Analysis calculations showed that although the dispersion is the most important component of energy of selenium-selenium interactions, electrostatic component is also very strong. Results also suggest that electrostatic component has crucial role in defining the geometry of selenium-selenium interactions. Reduced Density Gradient calculations on model systems showed that selenium-selenium interactions are often accompanied with additional C-H···Se interactions.

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References

1. S.P. Thomas, K. Satheeshkumar, G. Mugesh, T.N.G. Row, *Chem. Eur.J.* **2015**, 21,6793 –6800
2. J.S. Murray, P. Lane, P. Politzer, *Int. J. Quantum Chem.* **2008**, 108, 2770–2781.
3. I.S. Antonijević, G.V. Janjić, M.K. Milčić, S.D. Zarić, *Cryst. Growth Des.* **2016**, 16, 632–639