Sigma-hole bonding at R1-Se-R2 donors

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Abstract

Selenium has the possibility to form some non-covalent interactions, such as hydrogen and sigma-hole bondings like sulphur. A covalently-bonded selenium atom may have a region of significantly-positive electrostatic potential on its outer side, along the extension of a covalent bond. This is due to the electron-deficient outer lobe of a half-filled p-bonding orbital, so called “σ-hole.” The investigation with CSD data confirm that sigma hole bonding that involves Se exist in many structures, but quantum mechanics (QM) calculations show that sigma-hole involving Se is as stronger as the H-bonding, and is strictly oriented along sigma bond. In the same chemical environment, when substituted, the stability of the complex is in the following order: F > CN > Cl > Br > C=C, when ab-initio methods are used, and F > Cl > CN > Br > C=C following DFT methods, when NH3 and CH3OCH3 are employed as acceptors. However, with HCN as acceptor the stability sequence is in the following order: CN > F > Cl > Br.


Keywords: Sigma-hole bonding, selenium