

Poster Presentation

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Sigma -hole bonding at R1-Se-R2 donors

Albert Singa Lundemba¹

¹Kinshasa University, Kinshasa, Congo, Dem. Rep.

E-mail: albertlundemba@gmail.com

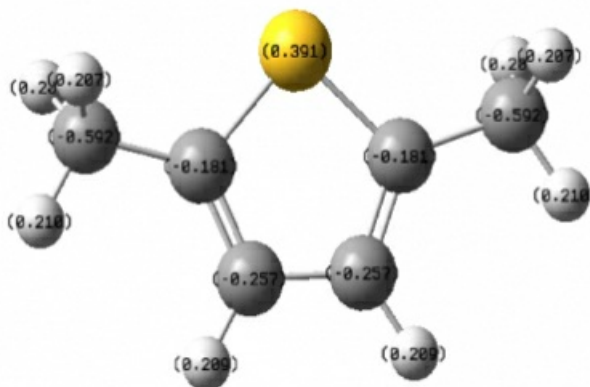
Lundemba Singaa, Bibelayi Dikimaa, Juliette Pradonb*, Anthony M. Reilly, Muswema L. Jeremiea, Colin R. Groomb, and Zéphyrin G. Yava *

a Département de Chimie, Université de Kinshasa, B.P.190 Kinshasa XI, République Démocratique du Congo. E-mail: albertlundemba@gmail.com. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.

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.

Dikima Bibelayi, Albert S. Lundemba, Frank H. Allen, Peter T. A. Galek, Juliette Pradon, Anthony M. Reilly, Colin R. Groom and Z'ephyrin G. Yav, Hydrogen bonding at C=Se acceptors in selenoureas, selenoamides and selones, Acta Cryst. (2016). B72, 317–325



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