

σ -Hole Bonding in Sulfur- and Selenium-Containing Heterocycles

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Abstract

In 1992, Temple Burling and Goldstein carried out a computational study focusing on nonbonded sulfur-oxygen and selenium-oxygen interactions in thiazole and selenazole nucleosides [1]. They used electrostatics to explain the conformational preference for the ether linkage of the ribose ring in these nucleosides to orient itself on the same side of the thiazole or selenazole ring bearing the sulfur or selenium. In this poster, we will show that this phenomenon can be explained in terms of σ -hole bonding [2-6], a highly directional noncovalent interaction between the electron deficient outer lobe of a half-filled p bonding orbital, called a σ -hole [2], and a nucleophile. Our computational tool for identifying these σ -holes is the molecular electrostatic potential, which we plot on molecular surfaces defined as the 0.001 electrons/bohr³ contour of the electronic density. In this poster we will explore the surface electrostatic potentials of some thiazoles, selenazoles and some other sulfur- and selenium-containing heterocycles, and we will show some interactions between these and selected nucleophiles.

References

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