

Noncovalent Interactions of Covalently-Bonded Group IV – VI Atoms

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Abstract

It has been known for more than half a century that covalently-bonded atoms of Groups IV – VI can interact with negative sites, in a highly directional manner, to form noncovalent complexes. Since 2007, it has been recognized that these are, in a great many instances, σ -hole interactions – and thus analogous to halogen bonding. A σ -hole is a region of diminished electronic density on a covalently-bonded atom. It is on the side of the atom opposite to a covalent σ bond, along the extension of that bond. If the electronic density is sufficiently reduced, a region of positive electrostatic potential can result, through which the atom can interact with negative sites. The attractive interaction is predominantly electrostatic/polarization, usually with a significant dispersion contribution. This presentation will discuss a number of examples of σ -hole bonding involving covalently-bonded atoms of Groups IV, V and VI.