

The Formation of σ -Hole Bonds: A Physical Interpretation

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The σ -hole was introduced into chemical jargon by Clark *et al* [1] just over ten years ago in Prague, at the Molecular Interactions in Biomolecules conference organized by Professor Jaroslav Burda. A σ -hole is due to the anisotropy of a covalently-bonded atom's electronic density along the extension of the covalent bond. In many instances this results in a region of positive electrostatic potential that can interact favorably with negative sites on other (or the same) molecules [2]. In this talk, the σ -hole concept will be shown to encompass many types of noncovalent interactions, including hydrogen bonding, halogen bonding and analogous interactions involving Group VI, V and IV covalently-bonded atoms [3]. The electronic densities of σ -hole bonds will be discussed in relation to (a) the approach of the interacting molecules, and (b) the resulting equilibrium complexes.

References

1. "Halogen bonding: The σ -hole"
T. Clark, M. Hennemann, J. S. Murray, P. Politzer, *J. Mol. Model.*, **13**, 291-296 (2007).
2. "Halogen Bonding and Other σ -Hole Interactions: A Perspective"
P. Politzer, J. S. Murray, T. Clark, *Phys. Chem. Chem. Phys.*, **15**, 11178–11189 (2013).
3. " σ -Hole Bonding: A Physical Interpretation"
P. Politzer, J. S. Murray, T. Clark, *Top. Curr. Chem.*, **358**, 19-42 (2015).