Research & Reviews: Journal of Chemistry

e-ISSN:2319-9849

EXPLORING HALOGEN BINDING MOTIIFS

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Editorial Note

Received date: 06/04/2021
Accepted date: 13/04/2021
Published date: 20/04/2021

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Keywords: Halogen, Mottifs, Lewis Base

EDITORIAL NOTE

The widespread and growing use of halogen bonding (XB) in various areas of life sciences, such as biomolecular engineering and drug development, highlights the need for a comprehensive understanding of the requirements and flexibility of this highly directed molecular interaction. The attraction of a partly positive region at the centre establishes XB as a non-bonded relationship. Halogen in extension of the R-X axis, where X is in most cases a chlorine, bromine or iodine atom and R is an electron withdrawing group, with an electron donor moiety, i.e., a π- or n-electronsIt's also worth noting that fluorine can undergo halogen bonding in very rare circumstances that are unlikely to be used in drug development. The electron configuration of the heavier halides may clarify this region of positive electrostatic potential, which is referred to as the -hole s2p2xp2yp1zs2px2py2pz1This positive area is usually surrounded by a negative belt in simple and symmetric molecules. Depending on the interaction partners, the binding energy of halogen bonding ranges from very weak to heavy ionically aided interactions (180 kJ/mol of ionic complexes). The form of halogen atom and the Lewis base (LB) are normally used to assess interaction hotspots, but they can also be measured by the type of halogen atom and the Lewis base (LB). Depending on the interaction partners, (180 kJ/mol of ionic complexes). While the type of halogen atom and the Lewis base (LB) are both important, interaction hotspots can usually be expected at a distance $d_{X\cdots LB}$ of ~2.75–3.5 Å and σ-hole angles $\alpha_{C-X\cdots LB}$ between 155 and 180.

The word "polar flattening" describes the non-spherically symmetric The magnitude, scale, linearity, and range of the -hole can all be used to describe it. The maximum electrostatic potential (ESP) value (called VS, max, or Vmax) found on the halogen surface with an electron density of 0.001 or 0.002 au is widely used to express the magnitude. 96–97% of the molecular charge is included at this electron density. The shape and magnitude of the -hole are influenced by different (hetero)aromatic ring systems as well as their substitution patterns. This effect is also known as “tuning”