

Studies on halogen bonding

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Halogen bond currently belongs to one of most intensively investigated noncovalent interactions. This is due to the fact that, similarly like in the case of hydrogen bond, it is relatively strong, directional and may play important role in various physical, chemical and biological processes. [1] The mechanism of formation of the halogen bond is rooted directly in anisotropy of electron charge distribution. Due to this anisotropy of charge density the halogen atom may exhibit dual character when it contributes in noncovalent interaction. It may act as both Lewis acid (in e.g. halogen bonding) and as Lewis base (in e.g. hydrogen bonding or another halogen bonding). Therefore, one may expect that in specific conditions the same halogen atom can interact *via* both such interactions, playing the role of Lewis base and Lewis acid, simultaneously. A few examples of such interactions will be presented. What is more, anisotropy of halogen atom was usually reported on the basis of analysis of various contacts observed in crystal state. [2] It will be shown that such observations may significantly depend on the molecular fragment used as a criterion in search through CSD. Thus, the analysis of electron density distribution around the halogen nucleus will be revisited. Finally some interesting cases of interactions, which can be considered as untypical halogen bonds, will also be presented.

[1] see e.g. A.C. Legon, Phys. Chem. Chem. Phys. 12:7736, 2010 and references therein.

[2] S.C. Nyburg, C.H. Faerman, Acta Cryst. B 41:274, 1985.