Poster

Application of quantum chemistry methods to analyse supramolecular architecture of halogen substituted anilines

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The halogen substituted anilines (Fig.1) are key structural blocks of bioactive products, medically important compounds and organic functional materials. Therefore, the study of molecular and crystal structure of such a type of compounds has an immense importance.All modern approaches to the molecular crystal structure analysis base on the comparison of the geometric characteristics of intermolecular interactions. However, these approaches are useless in many cases: a lot of weak interactions presence, the specific directed interactions absence etc.

In the case of halogen substituted anilines the presence only of weak (N/C-H…π, N-H...N and halogen bonds) types of intermolecular interactions complicates the description of the crystal structures. It is difficult to define the main structural motif in the solid state just on the basis of geometrical considerations. Taking into account the significant attention to halogen bonds in recent years, it is interesting to compare the crystal structures of the isomers of halogen substituted anilines from energetic viewpoint and analyze the role of different types of intermolecular interactions. The crystal packing analysis from energetic viewpoint indicates that the role of halogen bonds in supramolecular architecture depends on the position of halogen atom in the aromatic cycle.

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