Title:	Understanding of the Weak Intermolecular Interactions Involving Halogens in Substituted N-Benzylideneanilines: Insights from Structural and Computational Perspectives
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Abstract:	The C-F group, which is found in a large number of small organic molecules and drugs available in the market, has still not been fully understood in terms of the strength and directionality of the interactions offered by this group in guiding the formation of crystal lattices. In this manuscript, we have tried to understand the role played by the C-F group, using a model system of N-benzylideneanilines, on which we have previously done a systematic study with fluorine as a substituent on both rings. The effect on the packing of these molecules by replacing one of the fluorine atoms by either Cl or Br has been comprehended in this manuscript. It was observed that the features of the difluorinated analogues remained intact when the noninteracting fluorine atom was replaced by Cl or Br, while with the replacement of the interacting fluorine by Cl or Br, completely different packing characteristics were found to be developed. To quantify the strength of the interactions offered by "organic fluorine", stabilization energies of the dimers (which has been found to interact through the C-H···F hydrogen bond) have been calculated by Gaussian 09 at the MP2 level using a 6-31+G* basis set. These values were found to be between -0.3 and -6.0 kcal/mol. To study the topological properties of the interacting molecular pair, AIM calculations have also been done using AIM2000. In the studied dimers, the existence of bond critical points (BCPs) at the C-H···F hydrogen bond have always been seen and Laplacian at those BCPs has also been found to be positive, which is clearly an indication of a closed shell type of interaction between the C-H and F-C groups.
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