Title:	Structural investigation of weak intermolecular interactions in fluorine substituted isomeric N-benzylideneanilines
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Abstract:	The study of the influence of aromatic C-F group in directing crystal packing is an important area of current research. The role of the aromatic C-F group in the formation of weak intermolecular interactions in the absence of strong hydrogen bond donors and acceptors has been analyzed in a series of 15 newly synthesized fluorine substituted (mono- and di-) isomeric N-benzylideneanilines. It was observed that five compounds (out of a total number of 15) were liquids at room temperature, while others have low melting points (<60 °C). In situ crystallization, using an optical heating and crystallization device (OHCD), has been used to crystallize and determine the crystal structures of three out of five compounds which were found to be liquids at 25 °C. A detailed investigation of the molecular conformation and the crystal packing in these compounds reveals that the presence of organic fluorine acts as a significant contributor in the construction of various supramolecular synthons, essentially using a variety of C-H···F intermolecular interactions. These have been found to generate different three-dimensional arrangements of molecules in the crystalline framework. In order to realize the stabilizing influence exerted by such weak interactions, intermolecular C-H···F interaction energies have been calculated using Firefly to quantify the strength of such interactions. Lattice energy calculations have been performed and the individual energies, namely, the Coulombic, polarization, dispersion, and repulsive contributions to the lattice energy have been determined using the CLP program. In addition to these, theoretical calculations have been performed at the density functional theory level, and the experimental geometry has been compared with the optimized geometry to highlight the importance of molecular conformation in the solid and gas phase. It is of interest to note that stabilization resulting from the presence of C-H···F interactions, albeit less, is not negligible and does contribute toward crystal packing.
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