Experimental and computational insights into energy contributions of intermolecular interactions in fluorine & trifluoromethyl substituted N-phenylisobutyramides

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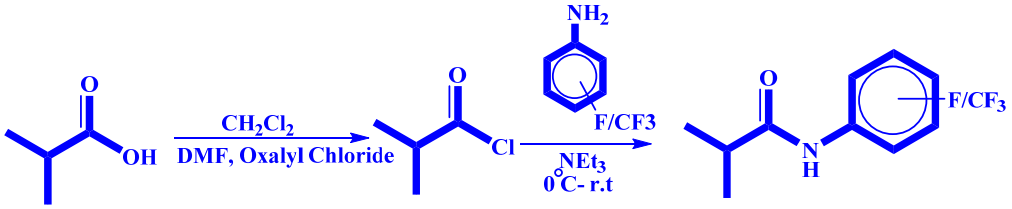
Abstract:

The presence of the C–F bond in organic molecules, particularly in the context of generating different intermolecular interactions of the type C–F···F–C, C–H···F–C and C–F···π is of extreme significance in the realm of structural chemistry[1]. These interactions generate different packing motifs in the formation of the crystal. It is of interest to evaluate the energetic contributions of such weak interactions to evaluate their important role in crystal packing[2]. In this respect, a library of seven compounds have been synthesized [Scheme 1] containing a strong donor (N–H) and a strong acceptor (C=O), and these have been characterized using ^{1}H NMR spectroscopy, single crystal X-ray diffraction, powder X-ray diffraction techniques, and their melting points were determined by DSC. In addition, the non-fluorinated counterpart has also been synthesized and characterized. A plethora of weak interactions, namely C(sp^2/sp^3)–H···F–C(sp^2/sp^3), C(sp^2/sp^3)–F···F–C(sp^2/sp^3) and C(sp^2/sp^3)–F···π are involved in crystal packing in addition to strong N–H···O=C hydrogen bonds[3] and weak C-H··· π and π···π contacts[4]. Detailed analyses of all the crystalline solids were performed with quantitative inputs from interaction energy calculations using the PIXEL method and a complete topological analysis were used to characterize these interactions.



Scheme 1: Synthesis of Fluoro and trifluoromethyl substituted N-phenylisobutyramides

References and Notes:

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