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Title:	Structural and Computational Analysis of Organic Fluorine-Mediated Interactions in Controlling the Crystal Packing of Tetrafluorinated Secondary Amides in the Presence of Weak C-H...O=C Hydrogen Bonds
Authors:	Singla, Labhini (/jspui/browse?type=author&value=Singla%2C+Labhini) Yadav, Hare Ram (/jspui/browse?type=author&value=Yadav%2C+Hare+Ram)
Keywords:	rganic Fluorine-Mediated Interactions Controlling the Crystal Packing Tetrafluorinated Secondary Amides Presence of Weak C-H...O=C Hydrogen Bonds
Issue Date:	2022
Publisher:	ACS Publications
Citation:	Crystal Growth and Design, 22(3), 1604-1622.
Abstract:	The structural and computational analysis of small organic compounds containing four fluorine atoms is the theme of this manuscript. A library of fluorinated compounds containing a secondary amide (-CONAr ₂) group has been synthesized and structurally characterized to understand the influence of multiple C-F bonds in building various supramolecular synthons. The introduction of four C-F bonds in each molecule has resulted into a variety of fluorine-mediated weak hydrogen-bonded synthons and a few C-F...F-C contact-mediated molecular dimers. These molecules offer the possibility of exploring the wide variation in crystal structures resulting from different types of weak interactions offered by organic fluorine (C-F group) connected to an aromatic ring. Herein, we intend to demonstrate the significance of those interactions using structural and computational methods.
Description:	Only IISER Mohali authors are available in the record.
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