Title:	Evaluation of fluorine-mediated intermolecular interactions in tetrafluorinated tetrahydroiso-quinoline derivatives: synthesis and computational studies
Authors:	Singla, L. (/jspui/browse?type=author&value=Singla%2C+L.) Yadav, H.R. (/jspui/browse?type=author&value=Yadav%2C+H.R.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Tetrahydroisoquinoline Organic fluorine Crystal engineering Structural analysis Energy computation
Issue Date:	2020
Publisher:	International Union of Crystallography
Citation:	Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 76, pp.604-617.
Abstract:	Intermolecular interactions involving the aromatic C-F group in the absence of other strong hydrogen bond acceptors is the theme of this article. Weak interactions involving fluorine are known to generate various supramolecular synthons, thereby altering the crystal structures of small organic molecules. It is demonstrated that the weak interactions involving organic fluorine play a major role in directing crystal packing of highly flexible organic molecules like diphenyl tetra-hydroisoquinolines reported herein. The intramolecular C-H···F hydrogen bonds are found to be significant in controlling the molecular conformation in specific cases wheras the intermolecular interactions involving the C-F groups result in a wide range of supramolecular synthons involving C-H···F and C-F···F-C interactions. The interactions are studied computationally to provide insight into their energies and the topology of the interactions is studied using Atoms in Molecules. C-H···F-C interactions are found to be quite stabilizing in nature with the stabilization energy of-13.9 kcal mol-1.
URI:	https://scripts.iucr.org/cgi-bin/paper?S2052520620006873 (https://scripts.iucr.org/cgi-bin/paper?S2052520620006873) http://hdl.handle.net/123456789/3197 (http://hdl.handle.net/123456789/3197)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/3197/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/3197?mode=full)
(/jspui/handle/123456789/3197/statistics)