Title:	Study of Halogen-Mediated Weak Interactions in a Series of Halogen-Substituted Azobenzenes
Authors:	Karanam, M. (/jspui/browse?type=author&value=Karanam%2C+M.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Weak interactions Understand Model compounds Azobenzenes
Issue Date:	2013
Publisher:	American Chemical Society
Citation:	Crystal Growth and Design, 13(11),pp. 4803-4814.
Abstract:	The azobenzenes, known for their various importance in the industry, have been chosen as model compounds to understand the role of weak interactions involving the C–X (X = F, Cl, and Br) bond using single-crystal X-ray diffraction technique, especially in the absence of other stronger intermolecular forces such as hydrogen bonds. The fluorinated compounds have been found to pack in the lattice by utilizing C–H···F hydrogen bonds, whereas the chlorinated and brominated analogues have been found to prefer C–X···X–C, C–X···π, and π···π interactions while packing in the lattice. The stabilization energy offered by the C–H···F hydrogen bonds and the C–X···X–C interactions have been estimated by computational methods using Gaussian 09, and the topological properties have been determined by using the AIM2000 package. The lattice energy decomposition has been done using semiclassical density sums (SCDS) PIXEL method. Our studies indicate that the stabilization energy offered by each C–H···F hydrogen bond lies in the range from −0.8 to −1.0 kcal/mol, while that for the C–X···X–C interaction has been found to be −0.35 kcal/mol for the X = Cl interaction and −0.73 kcal/mol for the X = Br interaction. Further, the analysis of these interaction by atoms in molecules (AIM) theory indicates that the electron densities (ρc) at the bond critical points (BCP) for C–H···F and C–X···X–C (X = Cl and Br), calculated using the AIM2000 package, are small (<0.007 eÅ–3), and the values of Laplacian (∇2ρc) are positive. This indicates that these interactions are of the hydrogen bond type. A detailed study of these interactions by experimental and computational methods has been described in the manuscript.
URI:	https://pubs.acs.org/doi/abs/10.1021/cg400967k (https://pubs.acs.org/doi/abs/10.1021/cg400967k) http://hdl.handle.net/123456789/2770 (http://hdl.handle.net/123456789/2770)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/2770/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/2770?mode=full)

(/jspui/handle/123456789/2770/statistics)