A Speculative Discussion of the Structural Details of 1-Bromo-2-iodo-benzenes

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The crystal and molecular structures of 2,4-dibromo-1-iodo-benzene (**1**) and 1,3-dibromo-2-iodo-benzene (**2**) have been determined by single crystal X-ray diffraction. The proximity of two or three large halogen substituents (Br/I) induces only minor distortions of the C-C-Br/I angles (*ca.* 2°) and the halogen atoms remain in the plane of the molecules. These undistorted structures lead to short intramolecular, sub-van-der-Waals Br–I contacts [in the range 3.465(4) to 3.530(4) Å]. The results suggest that the peripheral Br–I interactions have an attractive component which alleviates the repulsion out of steric crowding. The influence is associated with an absorption in the visible region and is possibly responsible for the enhanced reactivity of the 1,2-dihalobenzene molecules.

Key words: Bromobenzenes, Iodobenzenes, Bromo-/Iodo-Benzenes, Steric Crowding, Closed-shell Interactions