

MS23-01 Intermolecular halogen...halogen contacts in crystals with heteroatomic halogens. Olga V. Grineva, Chemistry Department, Moscow M.V. Lomonosov State University, Russia
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Intermolecular contacts with participation of halogen atoms are intensively studied during the last two decades [1]. Geometric parameters of the shortened (in comparison with the sum of van der Waals radii) contacts between the same halogen atoms are analysed since the early 1960s [2], and up to now almost all investigators are interested in the shortened contacts only. Meanwhile, it was noted in [3] that there were layers formed by the chlorine atoms in three polymorphs of *p*-dichlorobenzene. In our works [4-9], it was found that the halogen atoms had several neighbours in many other crystals, that lead to a formation of finite or infinite Hal-aggregates. Rather often some contacts in these aggregates were longer (up to 0.5 Å) than the sum of van der Waals radii, but the high probability of Hal-aggregation in crystals with the low halogen content [6] and in crystals with hydrogen bonds [9] testified their importance. In [5-9], homomolecular crystals with homoatomic halogens were investigated. In this work, crystals with heteroatomic halogens are retrieved from Cambridge Crystallographic Database, and the main attention is given to structures with two halogen atoms of two types (i.e., for example, with one fluorine and one chlorine *etc.*; about 1050 hits). Influence of a) types of halogen atoms, b) molecular structure (including molecular shape, positions of halogen atoms, presence of other functional groups) on the intermolecular Hal...Hal contacts and Hal-aggregation is discussed. For example, it is revealed that intermolecular I...I contacts in crystals with 1 F + 1 I are considerably less probable than in crystals with 1 Br + 1 I.

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MS23-02 Ten polymorphs of NH...N bonded DABCO hydroiodide - and even more! Anna Olejniczak and Andrzej Katrusiak, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland
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1,4-Diazabicyclo[2.2.2]octane hydroiodide (dabcoHI) is the first material for which anisotropic relaxor properties were reported.¹ The ferroelectric relaxors, possessing dielectric constant exceeding several thousands, are particularly desired for their numerous practical applications. They are required for miniature electronic devices, but most importantly, they can revolutionize the methods of storing electricity in capacitors. Organic relaxors are environment friendly and easier to produce and to dispose off than inorganic relaxors, which are mainly mixed perovskites and lead-containing ceramics. DabcoHI undergoes a large number of transformations at elevated pressure and temperature.² A subtle interplay of supramolecular aggregation, crystal symmetry, and bistable proton sites in NH...N hydrogen bonds in dabcoHI leads to the giant dielectric response in this compound. This unique feature disappears on increasing the temperature above 410 K or on increasing the pressure above 40 MPa at 296 K. In all the structures determined by X-ray diffraction so far, linear or nearly linear chains of cations are linked by NH⁺...N hydrogen bonds. The polymorphic structures differ mainly in the arrangement of the chains and iodide anions, in the dabco conformation, and in the location of protons. When crystallized from methanol, above 1.70(5) GPa, dabcoHI forms solvates. High-pressure crystallization from aqueous solution leads to hydration already at 0.50 GPa.³

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