

MS35-P28 | EVALUATION OF TRENDS IN A SERIES OF HALOGENATED ISOPHTHALAMIDES

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A series of halogenated isophthalamides (**X-DIPs**; **X** = halogen) has been synthesised and characterised by conventional spectroscopic techniques and single crystal X-ray diffraction. The series builds on previous studies of the crystal structures of benzamides and carboxamides together with their physicochemical properties, especially melting point analyses. Structural comparisons are made with results obtained from conformational analyses (potential energy scans) and modelled minima correlated with crystal structure data.

Structures in the **X-DIP** series preferentially adopt either the *anti-anti*- or *syn-anti* molecular conformations. In **Br-DIP**, molecules aggregate *via* reciprocal N-H...N and C-H...N interactions about inversion centres forming molecular pairs [graph sets $R^2_2(7)$, $R^2_2(20)$]. **Br-DIP** pairs connect by N-H...O and C-H...O interactions that cumulatively aggregate into a one molecule wide sheet (~20 Å wide) and parallel with the *bc* plane. Strong intermolecular interactions within the sheet involve both amides and pyridines (N-H...O=C; N-H...N), together with C-H...O/N interactions. Two sheets form per unit cell intersecting at $x = 0, 0.5$. The sheet surface contains Br atoms interspersed regularly as an array with five shortest Br...Br distances from 4.1 to 5.1 Å. Sheets link by Br...Br halogen bonding with shortest Br...Br = 3.6197(17) Å. Two other Br...Br contacts span the sheet interface at 3.8534(14) Å and 3.8988(16) Å. The sheet surface does not contain any other type of intermolecular interaction and one can surmise that sheets can glide over one another easily and may explain the observed twinning.