

Secondary Bonding Interactions in Some Di- and Trihaloanilinium Halides

Esperanza López-Duplá, Peter G. Jones, and Fabiola Vancea

Institut für Anorganische und Analytische Chemie, Technical University of Braunschweig,
Postfach 3329, D-38023 Braunschweig, Germany

Reprint requests to Prof. P. G. Jones. E-mail: p.jones@tu-bs.de

Z. Naturforsch. **58b**, 191 – 200 (2003); received October 18, 2002

Six solvent-free structures of di- and trihaloanilinium halides are presented. All involve clearly defined hydrophilic regions built up from classical hydrogen bonding systems. The 2,4-dibromo-, 2,6-dichloro-, 2,4,6-trichloro- and 2,4,6-tribromoanilinium derivatives form ribbon structures involving annelated $R_4^2(8)$ rings with NH_2 donors (two hydrogens from the positively charged NH_3 groups) and halide acceptors. The 2,5-dibromo- and 2,4,5-trichloro derivatives form layers with two types of ring, $R_4^2(8)$ and $R_8^4(16)$. All structures also involve other secondary interactions (C-H...X hydrogen bonds and/or X...X contacts, X = halogen), some of which link the ribbons or layers into a second or third dimension. The shortest X...X contacts generally involve the anions. In the 2,4-dibromo, 2,4,6-trichloro and tribromo derivatives, somewhat more extensive halogen aggregates (triangles, angled X_3 or X_4 chains) are formed between neutral halogens. In two appendices, the packing patterns of (I) the disordered structure 3,4,5-trichloroanilinium chloride and (II) the known structures of unsubstituted anilinium halides are briefly presented.

Key words: Anilinium, Halides, Hydrogen Bonds, Halogen-Halogen Contacts