Secondary Bonding Interactions in Some Dichloroanilinium Chlorides

Lilian Gray and Peter G. Jones

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

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

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Of the six structures presented here, five involve clearly defined hydrophilic layers built up from classical hydrogen bonding systems. Of three solvent-free structures, 2,4- and 3,5-dichloroanilinium chlorides both form ribbon structures involving annelated \( R_2^2 \) rings with \( \text{NH}_2 \) donors (two hydrogen atoms from the positively charged \( \text{NH}_3 \) groups) and chloride acceptors. The ribbons are linked by weaker interactions to form layers. 2,5-Dichloroanilinium chloride forms a layer structure directly, with rings \( R_3^3 \) exactly analogous to those previously observed in 2-chloroanilinium chloride. 2,6-Dichloroanilinium chloride methanol solvate forms a different type of ribbon structure, with alternating \( R_2^2 \) and \( R_4^4 \) rings; the latter involve two chlorides, two \( \text{NH}_2 \) groups and two methanols. These ribbons too are linked to form layers. 2,3-Dichloroanilinium chloride hydrate forms layers with two types of ring \( R_3^3 \); one involves two \( \text{NH}_2 \), two chlorides and the OH part of a water, whereas in the other, an \( \text{NH}_2 \) is replaced by \( \text{OH}_2 \). In all these structures the aromatic groups project approximately perpendicular to the layers to form hydrophobic regions; for all except 3,5-dichloroanilinium chloride, neighbouring layers are linked by weaker interactions such as C-H--Cl hydrogen bonds or Cl--Cl contacts. The final structure, 3,5-dichloroanilinium chloride 1/4-hydrate, is completely different; it involves two types of columns, one built up from quadrilaterals of Cl--Cl contacts between cations and the other consisting of “nanotubes” of \( \text{NH}_3 \) groups and chloride anions linked by two- and three-centre hydrogen bonds. The columns are in turn linked by cation-anion Cl--Cl interactions.