Synthesis and Structural Characterization of Diisopropylammonium Trifluoroacetate and Diisoproplyammonium Pentafluoropropionate

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Diisopropylammonium trifluoroacetate ([{iPr₂NH₂][CF₃COO]}]; dip tfa; 1) and diisopropylammonium pentafluoropropionate ([{iPr₂NH₂}[C₂F₅COO]}]; dip pfp; 2) have been synthesized and structurally characterized by X-ray diffraction and spectroscopic methods. Both compounds form hydrogen-bonded cyclic dimers (Etter symbol: \(R_4^4(12)\)) in the solid state. The asymmetric unit of 1 contains one trifluoroacetate anion and one dip cation in the centrosymmetric space group \(P\bar{1}\). The asymmetric unit of 2 consists of two crystallographically independent pentafluoropropionate anions and two independent dip cations forming dimers in the form of rings, both lying around centers of symmetry in the space group \(P\bar{1}\). In dip tfa and dip pfp the cations act as double hydrogen bond donors, and each of the two oxygen atoms of the carboxyl group are single hydrogen bond acceptors. The donor acceptor distances of the N–H⋯O hydrogen bonds are within the expected range for medium strong hydrogen bonds. The quasi-molecular cyclic dimers are connected with neighboring units only by van der Waals interactions.

Key words: Diisopropylammonium Cation, Hydrogen Bonding, Crystal Engineering, Carboxylates