

Poster Presentations

[MS25-P06] Hydrogen-bonding in a new fluorosilicate salt based on phenylalaninium

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Fluorosilicate salts involving onium cations of N-- and O-- containing organic bases and amino acids have practical applications as ionic liquids (Katayama et al., 2001), dielectrics with cryptocrystalline structure (Kalem, 2004) and layered organic-inorganic hybrid materials (Airoldi & De Farias, 2000). This new hybrid compound has been prepared by slow evaporation of an aqueous solution of phenylalaninium, SiO₂ and hydrofluoric acid in a molar ratio of 10:5:1. The asymmetric unit of compound II is built up from a (+/-)-phenylalaninium cation and half a molecule of hexafluorosilicate anion located on inversion center, connected by N-H...F hydrogen bonds. All the F atoms of the hexafluorosilicate anion act as acceptors and are engaged in N-H...F and O-H...F bondings with the alaninium part of the cation. Two H atoms and their symmetry related counterparts (x, -y, 1-z), of the ammonium NH₃⁺ interacts with two symmetry₄ related fluorosilicate (-x, -y, 1-z) building a R₂(8) ring whereas, the third H atom of the NH₃⁺ and the H atom of the symmetry related (-x, y+1/2, -z+1/2) carboxylate complete a R₃(10) graph set motif. These hydrogen bonds result in the formation of layers parallel to the (1 0 0) plane. In these layers, chains of cations and anions alternate. The phenyl rings of the symmetry related layers are intercalated, however the centroid to centroid distance between the phenyl rings are too long (4.958(1) and 4.523(1) Å) for considering π - π interactions.

[1] Katayama, Y., Yokomizo, M., Miura, T. & Kishi, T. (2001). *Electrochemistry*, 69, 834-836.

[2] Kalem, S. (2004). *Appl. Surf. Sci.* 236, 336-341.

[3] Airoldi, C. & De Farias, R. F. (2000). *J. Fluorine Chem.* 103, 53-55.

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