CRYSTAL STRUCTURES AND SOLUBILITY OF 4,4′-BIPYRIDINIUM AND 2-BROM-5-METHYLPYRIDINIUM HEXAFLUOROSILICATES

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Hexafluorosilicates with heterocyclic cations are convenient models for the estimation of H-bonds influence on structural characteristics and properties of this onium salts. As a part of our systematic investigation here we describe results of X-ray structure analysis and solubility data determination of the hexafluorosilicates (4,4′-DipyH2)SiF6 (I) and (2-Br-6-CH3C5H3NH2)2SiF6·H2O (II).

Colourless crystals of the compounds I and II were separated as products of the interaction of hexafluorosilicic acid with corresponding amine. Crystal structures of I and II (a, c) and fragments of crystal packing in I and II (b, d) are presented below.

Both structures are built from the H-bonded units consisting of the SiF62− anion and cations. Structure II also includes the water molecule. Complex I represents example of the structure in the form of 1D chain, in which 4,4′-DipyH22+ cations and SiF62− anions joined through strong N(1)H⋯F(3) bonds (N⋯F 2.694(2) Å). In the SiF62− anion the Si–F bond lengths are between 1.6749(11) and 1.7054(10) Å. The fluorine atoms in the longer Si(1)–F(3) bond participates in the H-bond. The crystal structure II is stabilized by the network of H-bonding O(1W)H⋯F(1) (O⋯F 2.805(8) Å), O(1W)H⋯Br(1) (O⋯Br 3.00(4) Å), O(1W)H⋯F(3) (O⋯F 2.779(7) Å), N(1)H⋯O(1W) (N⋯O 2.709(9) Å).

The solubility data of I, II and (2,2′-DipyH2)SiF6 (III) in water (mol. %, 25 °C): 0.36, 2.01, 10.58. Some relationship between solubility data and interionic H-bonds characteristics of onium hexafluorosilicates will be discussed.