P33

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

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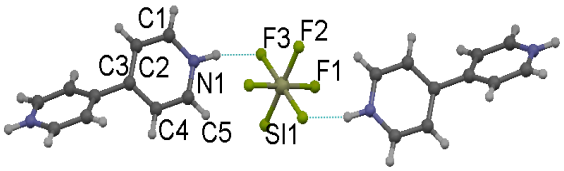
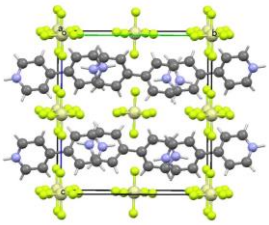
Hexafluorosilicates with heterocyclic cations are convenient models for the estimation of H-bonds influence on structural characteristics and properties of this onium salts. As a part of our systematic investigation here we describe results of X-ray structure analysis and solubility data determination of the hexafluorosilicates (4,4′-DipyH_2)SiF_6 (**I**) and (2-Br-6-$CH_3C_5H_3NH)_2SiF_6 \cdot H_2O$ (**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.



a



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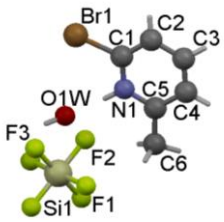
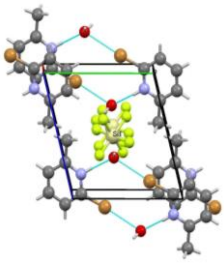


c



d

Both structures are built from the H-bonded units consisting of the SiF_6^{2-} 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′-DipyH_2^{2+} cations and SiF_6^{2-} anions joined through strong N(1)H···F(3) bonds (N···F 2.694(2) Å). In the SiF_6^{2-} 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′-DipyH_2)SiF_6 (**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.