

Letter to the Editor

A Novel Clathrate Hydrate Structure of Tetra-Iso-amyl Ammonium Fluoride

JANUSZ LIPKOWSKI* and KINGA SUWIŃSKA,

Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01224 Warszawa, Poland

K. UDACHIN, T. RODIONOVA, and YU. DYADIN

Institute of Inorganic Chemistry, USSR Academy of Sciences, Siberian Branch, 630090 Novosibirsk, U.S.S.R.

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In the phase equilibria studies of the systems: water/tetraalkylammonium fluorides, a distinct solid phase has been found of composition $C_{20}H_{44}NF/26.7 H_2O$. A single crystal of the compound was used for X-ray structure determination at $-50^\circ C$. The lattice parameters are: $a = b = 16.894(5)$, $c = 17.111(2)$ Å, space group $I4_1/a$, $Z = 8$. Solution of the structure reveals a new polyhedral structure of the host cavities, as shown in the Figure. The structure is now refined to $R = 0.072$ for 1158 observed reflections used in the calculations.

The cavity shown in the Figure has $\bar{4}$ symmetry and may be seen to be rather a strained one since there are eight square faces at the connections between the four 'subcavities' which accommodate one iso-amyl group each. These parts have 3 hexagonal, 7 pentagonal and two square external faces.

The fluoride anion has not yet been localized – it seems it is included in the host framework and is disordered within it.

A full paper on this interesting structure will be submitted soon, after completion of the analysis of the X-ray diffraction data – the present report is based on little more than half of the full data set.

* Author for correspondence.

