The crystal structure of KAsF₆. By RAYMOND B. ROOF JR., *Mineralogical Laboratory, University of Michigan, Ann Arbor, Michigan, U.S.A.*

Potassium arsenic hexafluorine is the first of an extensive series of arsenic–fluorine compounds being prepared for investigation by the Chemistry Department at the University of Michigan. The purpose of the investigation of the crystal structure of $KAsF_6$ was to establish the interatomic distance between As and F and to examine the role of K in the bonding of the crystal.

Minute single crystals were grown from a water solution and these crystals exhibited the symmetry $\bar{3}$. Weissen-

Table 1. *Comparison of observed and calculated powder line intensities*

(Cu $K\alpha$ radiation)

Line No.	θ (°)	$hk.l$	$F_{O}^2 p$	$F_{c}^2 p$
1	9·2	10.1	30	25
2	12·1	11.0	69	82
3	14·1	01.2	72	61
4	15·3	02.1	27	33
5	18·7	00.3, 20.2	27	30
6	19·7	21.1, $\bar{2}3.1$	15	8
7	21·3	30.0	21	19
8	22·6	12.2, 11.3, $\bar{1}2.3$, $\bar{1}3.2$	228	285
9	24·8	22.0	48	67
10	26·1	10.4	24	25
11	26·7	13.1, $\bar{1}4.1$	42	34
12	29·0	$4\bar{1}.2$, 03.3, 31.2, 30.3, 02.4	105	113
13	32·0	04.2, 22.3, 21.4, $3\bar{1}.1$	198	155
14	32·6	32.1, $5\bar{2}.1$	24	28
15	33·7	41.0, 14.0	78	72
16	34·6	23.2, $\bar{2}5.2$, 01.5	81	69
17	35·5	20.5	15	18
18	37·4	05.1, 13.4, $\bar{1}4.4$	54	36
19	39·0	33.0, 12.5, $\bar{1}3.5$	63	86
20	39·8	00.6, 50.2, 41.3, 14.3	90	97

berg photographs established the space group as $R\bar{3}$. The hexagonal unit cell lattice constants are

$$a = 7.352, \quad c = 7.235 \text{ Å} .$$

From a measured density of 3·29 g.cm.⁻³ the number of formula weights per unit cell was determined as $Z = 3$. Intensity measurements were made by a photodensitometer trace of a powder photograph of the material which was taken with Cu $K\alpha$ radiation.

Table 1 compares the observed and calculated powder line intensities. The observed intensities have been corrected for the Lorentz and polarization factors. The factor p is the multiplicity factor. An experimentally determined temperature factor, $B = 0.7$ Å², was applied to the calculated intensities. The interpretation of the powder photograph is also given.

The crystal structure of $KAsF_6$ can be described as follows:

$$(0, 0, 0), \ (\tfrac{1}{3}, \tfrac{2}{3}, \tfrac{2}{3}), \ (\tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{3})+$$

  1 As at 0, 0, 0;
  1 K at 0, 0, $\tfrac{1}{2}$;
  6 F at x, y, z etc.,

where

$$x = 0.117, \quad y = 0.234, \quad z = 0.152 .$$

These coordinates were determined from Fourier projections on 00.1 for x and y and $\bar{1}2.0$ for z. The As–F distance was determined to be 1·85 Å. The value of the residual computed from the structure factors is $R = 0.19$.

The six F atoms are arranged in a very slightly distorted octahedral coordination around the arsenic atom. The attractive forces of the K atom have caused the F atoms to move parallel to the 111 direction of the octahedron so that the F–As–F angle is reduced to 88°. The structure can be compared to that of an ideal simple cubic structure (the AsF_6 groups at the corners of the cube and the K atom at the center of the cube) in which the attractive forces of the K atom have reduced the c/a ratio of the ideal cubic by 20%.

Crystallographic data for dioxospartalupine hydrate, C₁₅H₂₂N₂O₂.H₂O.* By A. E. LESSOR, JR.,† *Chemistry Department, Indiana University, Bloomington, Indiana, U.S.A.*

Crystals grown from a solution in hot n-hexane were long needles with well formed pinacoids {001}. Precession and Weissenberg photographs were taken with the crystal

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mounted parallel to the needle axis, and gave the orthorhombic unit-cell dimensions:

$$a = 6.19, \quad b = 10.39, \quad c = 21.92 \text{ Å} .$$

There are four molecules per unit cell. Density: calculated 1·32 g.cm.⁻³; observed (flotation) 1·28 g.cm.⁻³.

Reflections of types $(h00)$, $(0k0)$ and $(00l)$ were ob-