Vol. A53 (1978) *ACTA PHYSICA POLONICA* No 5

LATTICE CONSTANTS, SPACE GROUPS AND POWDER DATA FOR $UO_2SO_4 \cdot 2CO(NH_2)_2$ AND $UO_2SO_4 \cdot 3CO(NH_2)_2$ CRYSTALS

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(Received March 23, 1977; Revised version received November 3, 1977)

The lattice parameters and space groups for two intermolecular compounds of urea with uranyl sulphate was determined using X-ray crystallography experimental methods.

1. Introduction

Urea forms many crystalline intermolecular compounds with various inorganic compounds, also with compounds of uranyl ions [1]. The uranyl salts and urea form compounds of the general formula $UO_2X_2 \cdot mCO(NH_2)_2 \cdot pH_2O$ ($X = Cl^-$, J^-, CNS^-, ClO_4^-, NO_3^-, OH^-, $1/2SO_4^{--}$, $1/2CrO_4^{--}$; $m = 1 \div 6$; $p = 0$ or 1) [2–5].

In this paper lattice constants, space groups and powder data for the compounds of urea and uranyl sulphate with chemical formulas: $UO_2SO_4 \cdot 2CO(NH_2)_2$ and $UO_2SO_4 \cdot 3CO(NH_2)_2$ are given as determined by X-ray crystallography methods.

2. Experimental and results

The crystals of the urea intermolecular compounds with uranyl sulphate were obtained by evaporation at room temperature [6,7] of aqueous solutions of arbitrary concentrations, but containing uranyl sulphate and urea at molar ratios: 1:2 (and also 1:0.5, 1:1, 1:1.5)

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for $UO_2SO_4 \cdot 2CO(NH_2)_2$, and 1:3 (and 1:5, 1:10, 1:30 too) for $UO_2SO_4 \cdot 3CO(NH_2)_2$. The chemical analyses confirmed the composition indicated.

The $UO_2SO_4 \cdot 2CO(NH_2)_2$ crystals are yellow, and have prismatic form. The $UO_2SO_4 \cdot 3CO(NH_2)_2$ crystals with a yellow-greenish color, have the form of a rectangular plate. The crystals of both compounds are non-hygroscopic.

The densities of the crystals investigated were measured by the pycnometric method in paraffinum liquidum, at temp. 20°C.

For determination of the unit cell dimensions and space groups the crystals were examined by Laue, de Jong-Bouman and Weissenberg methods.

The powder diffractograms of the crystals examined were made on the URS-50-IM X-ray diffractometer with NiK_α radiation. Indexing of lines on powder diffraction patterns were calculated using an interplanar spacing formula.

The crystallographic data of the crystals examined are given in Table I.

The powder data for these crystals are listed in Table II.

TABLE I

Crystallographic data for the crystals examined

	$UO_2SO_4 \cdot 2CO(NH_2)_2$	$UO_2SO_4 \cdot 3CO(NH_2)_2$
C. S.	monoclinic	monoclinic
a(Å)	6.70±0.01	7.61±0.01
b(Å)	14.05±0.04	24.61±0.04
c(Å)	11.27±0.05	6.91±0.01
β	106.1°±0.5°	90.4°±0.5°
V(Å^3)	1019±6	1294±6
M	486.20	546.26
D(g/ccm)	3.21	2.74
D_x(g/ccm)	3.17	2.80
Z	4	4
Obs. refl.:		
hkl	no systematic absences	no systematic absences
$h0l$ for	$l = 2n$	$h+l = 2n$
$0k0$ for	$k = 2n$	$k = 2n$
S. G.	$P2_1/c$	$P2_1/n$

C. S. — crystallographic system; a, b, c, β — lattice parameters; V — volume of the unit cell; M — molecular mass; D — measured density; D_x — theoretical density; Z — number of stoichiometric molecules in the unit cell; Obs. refl. — observed reflections; S. G. — space groups.

TABLE II

Powder diffraction data for crystals examined

$UO_2SO_4 \cdot 2CO(NH_2)_2$				$UO_2SO_4 \cdot 3CO(NH_2)_2$			
d_{obs}(Å)	I_{obs}	hkl	d_{calc}(Å)	d_{obs}(Å)	I_{obs}	hkl	d_{calc}(Å)
8.54	100	011	8.56	6.47	61	120	6.48
7.03	27	020	7.02	6.18	100	040	6.15
5.88	67	110	5.85	5.58	7	130	5.58
		021	5.89	5.11	16	101	5.10
5.43	67	002	5.40	4.35	7	131	4.33
5.06	50	012	5.05	4.09	6	060	4.10
4.87	18	$\bar{1}02$	4.86	3.93	27	141	3.92
4.72	47	120	4.74	3.80	9	200	3.80
		$\bar{1}21$	4.71	3.62	35	220	3.63
4.64	54	111	4.67	3.55	15	170	3.52
4.30	44	031	4.30			151	3.53
		022	4.28	3.45	13	002	3.45
4.06	28	121	4.06	3.23	24	240	3.24
3.80	13	$\bar{1}31$	3.82	3.20	16	221	3.21
3.67	7	102	3.66	3.08	27	080	3.08
3.52	14	040	3.51			231	3.08
		013	3.49	3.02	19	042	3.01
		112	3.54	2.910	4	132	2.930
3.40	14	131	3.40			241	2.926
3.25	44	$\bar{2}11$	3.27	2.819	6	142	2.794
		122	3.25			260	2.790
3.22	94	200	3.21	2.644	10	181	2.634
		$\bar{1}23$	3.20	2.589	12	202	2.550
3.08	41	140	3.08			190	2.572
		$\bar{2}12$	3.10	2.489	7	0.10.0	2.460
2.920	8	220	2.925	2.394	23	301	2.374
2.872	38	132	2.889	2.349	11	242	2.355
		$\bar{2}22$	2.895			340	2.345
2.801	16	211	2.816	2.325	9	321	2.332
2.730	36	004	2.702	2.296	5	013	2.293
		$\bar{2}31$	2.722	2.266	4	281	2.258
2.663	34	014	2.657	2.229	5	341	2.213
		221	2.659	2.206	7	103	2.200
2.602	13	123	2.624			033	2.210
2.526	15	310	2.526	2.186	5	113	2.190
2.442	29	212	2.441	2.158	5	123	2.165
		231	2.449			262	2.165
2.420	18	$\bar{2}33$	2.416	2.064	6	0.12.0	2.050
		133	2.422			143	2.071
2.344	8	222	2.335	1.981	3	332	1.977
		060	2.340	1.968	8	213	1.957
2.279	3	104	2.279			223	1.957
2.230	13	$\bar{3}02$	2.215	1.939	5	342	1.937

TABLE II (continued)

$UO_2SO_4 \cdot 2CO(NH_2)_2$				$UO_2SO_4 \cdot 3CO(NH_2)_2$			
d_{obs}(Å)	I_{obs}	*hkl*	d_{calc}(Å)	d_{obs}(Å)	I_{obs}	*hkl*	d_{calc}(Å)
2.202	15	160	2.200	1.906	6	233	1.910
2.157	17	062	2.150			400	1.900
2.130	18	$\bar{3}21$	2.121	1.878	2	420	1.878
		300	2.143			243	1.871
2.072	13	320	2.051	1.816	6	440	1.817
2.036	16	242	2.020	1.808	6	421	1.811
1.998	11	$\bar{3}23$	2.002	1.719	7	004	1.720
		$\bar{3}32$	2.005			303	1.700
1.978	13	311	1.979				
1.957	8	321	1.957				
		330	1.950				
1.921	11	$\bar{3}33$	1.930				
1.889	19	071	1.881				
1.847	13	331	1.841				
1.829	13	204	1.830				
1.820	22	302	1.827				
1.801	28	006	1.801				
1.764	42	080	1.755				
1.750	13	$\bar{2}26$	1.745				
1.709	4	332	1.702				

d_{obs} — observed interplanar spacings, d_{calc} — calculated interplanar spacings, I_{obs} — observed relative intensities, *hkl* — diffraction indices.

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