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X-RAY DIFFRACTION STUDY OF $M_2Zn(TeO_3)_2$ (M - Na, K) TELLURIDE

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Abstract. The binary zinc telluride with the s-elements were synthesized by solid-phase method from the tellurium (IV) oxides, zinc and sodium (potassium) carbonates. The types of symmetry, unit cell parameters, X-ray and pycnometric densities of the synthesized compounds were determined by X-ray analysis.
Keywords: binary zinc telluride; solid phase synthesis; X-ray

Rare and trace elements play increasingly important role in modern technology, so the methods of obtaining and studying the properties of different compounds with unique physical and chemical properties are given much attention. Tellurium occupies an important place among the rare elements used in modern technology. Establishing the relationship between composition, structure and properties of materials is one of the most important problems in modern inorganic chemistry.

Knowledge of the relationship of structure and properties allows systematizing and predicting the existence of compounds possessing desired properties. Of course, in order to do this, we need comprehensive data on systematic studies of certain classes of chemical compounds.

Studies of perspective materials on the electrical properties have shown that the electrical parameters of complex oxides are determined not only by complex chemical composition, but also by the phase composition and structure of the crystal lattice. The stoichiometry of the phases and the symmetry of their crystal lattices depend on the elements that make up the matter. Information about the preparation of new compositions based on oxides of alkali, alkaline-earth, d-metals and tellurium is still little known. Oxide materials are currently the most common ones in modern electronics and microelectronics technology.

Telluride is coordination compound which have found application in chemical engineering, namely in production of glass, ceramics, construction materials and in physics as valuable compounds with the magnetic and electrical properties, and as optical and thermionic materials.

The aim of this work is the synthesis and study of X-ray properties of the new binary telluride of some s-d-elements.

TeO_2 marked as “extra pure”, ZnO and alkali metal carbonates marked as «chemically pure» were used for the synthesis of binary telluride. Samples of the starting materials were weighed up to four decimal places. Stoichiometric amounts of starting materials were carefully triturated into an agate mortar. Then, the samples were quantitatively powdered into a crucible and subjected to heat treatment for solid-phase interaction in an air furnace. We used the following mode of heat treatment: annealing for 25 hours at a temperature of 400 – 800 ^{0}C with periodic grinding in a mortar and then annealing was carried out at 400 ^{0}C for 15 hours in order to obtain stable compounds at low temperatures.

The formation of the compounds equilibrium composition was monitored by X-ray diffraction analysis on DRON - 2.0 using CuK α - radiation filtered with Ni-filter (U = 30 kV, J = 10 mA, the rotational speed is 1000 pulses per second, the time constant $\tau = 5$ sec, the interval of angles 2θ is from 10 to 90^0). The intensity of diffraction peaks was assessed by 100 points scale. Indexing of the compounds powder roentgenograms was performed by homology (Koyba & Trunov, 1976).

Indexing reliability is controlled by satisfactory coincidence of experimental and calculated values ($10^4/d^2$), as well as the consistency of the X-ray and pycnometric densities values of the compounds investigated. The tetrabromoethane of analytical grade placed into the 1.00 mL-pycnometer was used as an indifferent liquid in determining the phase pycnometric density. In this series the following operations were carried out: determination of the empty pycnometer mass (M_0), then the mass of pycnometer filled with distilled water (M_1), mass of pycnometer filled with tetrabromoethane (M_2); the test compound is then placed into the pycnometer

and the mass is determined as the dry matter (M_3), and finally powder is filled with pycnometric liquid and mass is measured (M_4). The density of the sample is given by:

$$\rho_{pycn.} = \frac{M_3 - M_0}{\frac{M_1 - M_0}{\rho_1} - \frac{M_4 - M_3}{\rho_2}} \quad (1)$$

where, ρ_1 is density of water at 20^0C (0.9971 g/cm^3); ρ_2 is the liquid pycnometric density found by Eq. (2):

$$\rho_2 = \frac{M_2 - M_0}{M_1 - M_0} \cdot \rho_1 \quad (2)$$

X-ray density ($\rho_{X\text{-}ray}$) of the compounds was calculated by Eq. (3):

$$\rho = \frac{1,66 \cdot M_r \cdot Z}{V^0} \quad (3)$$

where M_r is the molecular mass of the substance, Z is the number of formula units and V^0 is the volume of the cell.

The volume of the unit cell (V^0) of the compounds was determined by the Eqs. (4-7):

$$V^0 = a^3 \quad (4)$$

(for the cubic crystal system),

$$V^0 = a^2 \cdot c \quad (5)$$

(for the tetragonal crystal system),

$$V^0 = 0,86 \cdot a^2 \cdot c \quad (6)$$

(for the hexagonal crystal system) and

$$V^0 = a \cdot в \cdot c \quad (7)$$

(for the orthorhombic crystal system).

Table 1 shows the results of the powder indexing of the compounds studied. Satisfactory agreement between experimental and calculated values $10^4/d^2$ listed in Table 1, as well as the consistency of the values of x-ray and pycnometric density of the investigated compounds (Table 2) confirm the correctness of the compounds studied roentgenograms indexing performed.

Table 1. Roentgenograms indexing of binary tellurides

I/I_0	d, Å	$10^4/d^2$ exper.	hkl	$10^4/d^2$ calcul.
1	2	3	4	5
$Na_2Zn(TeO_3)_2$				
13	7.1556	195	100	196
1	2	3	4	5
17	5.5782	321	001	324
18	5.0765	388	011	396
29	4.4060	515	101	519
22	4.1494	581	111	592
9	3.9406	644	030	653
27	3.5796	780	200	783
10	3.4512	840	130	849
100	2.9381	1158	040	1161
32	2.7789	1295	002	1295
9	2.7341	1338	140	1356
30	2.6430	1432	230	1436
7	2.3928	1742	231	1759
22	2.2835	1918	240	1944
5	2.2136	2041	220	2051
7	2.1633	2137	51	2138
6	2.1120	2242	132	2144
9	2.0432	2395	321	2375
15	1.9171	2721	232	2731
20	1.7872	3131	400	3131
32	1.7643	3213	023	3204
15	1.7322	3333	322	3346
7	1.6480	3682	203	3697
33	1.6354	3740	421	3745
22	1.6239	3792	430	3784
13	1.4676	4643	080	4643
23	1.4203	4957	323	4965
7	1.3639	5376	104	5376
$K_2Zn(TeO_3)_2$				
21	5.120	382	101	381
1	2	3	4	5
15	4.230	559	132	531
14	4.010	622	051	610
9	3.640	755	20	755
12	3.268	936	201	947
16	3.180	989	161	982
100	3.070	1061	080	1068
22	2.977	1128	132	1108

16	2.940	1157	250	1172
10	2.840	1240	142	1225
15	2.810	1266	081	1260
6	2.690	1382	152	1375
19	2.630	1446	181	1449
9	2.540	1550	261	1548
22	2.430	1694	300	1698

As seen from Table 1 the value of the experimental and calculated values ($10^4/d^2$) of X-ray and pycnometric densities (Table 2) agree well with each other, which confirms the reliability and correctness of the indexing results. It also suggests that the compounds $Na_2Zn(TeO_3)_2$ and $K_2Zn(TeO_3)_2$ have the orthorhombic symmetry type and the unit cell parameters listed in Table 2.

Table 2. Types of symmetry and unit cell parameters of the telluride

Compound	Type of symmetry	The lattice parameters, Å			V0, Å3	Z	density, g/cm3	
		a	b	c			X-ray.	pycn.
Na2Zn(TeO3)2	rhombic	7.15	11.74	5.56	466.71	8	4.86	4.75 ± 0.12
K2Zn(TeO3)2	rhombic	7.28	24.48	7.21	1284.9	8	2.68	2.61 ± 0.08

Based on the data presented it can be stated that for the first time zinc binary telluride with s-elements were synthesized by the solid-phase method. Types of their symmetry and the unit cell parameters were determined by X-ray analysis. The X-ray studies show that the synthesized compounds crystallize in the P_m3_m structure type of distorted perovskite. Radiographic parameters of the new s-d-elements telluride are the baseline data for inclusion in the databases.

REFERENCES

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