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Synthesis, X-ray and quantum-chemical investigations of double tellurites of holmium

Complex oxide phases, namely new double tellurites of holmium with the composition $HoMe^{II}TeO_{4.5}$ (where Me^{II} — Sr, Ba) were synthesized with the ceramic technology from Ho(II), Te(IV) oxides and carbonates $SrCO_3$, $BaCO_3$ in the range of 800–1200 ºC. For the first time the structure of tellurites was investigated by X-ray phase analysis. X-ray phase analysis was performed on the DRON-2.0 device. The intensity of the diffraction peaks was estimated on a stable scale. Radiographs of the synthesized powders were indicated by the homology method. The type of syngony, unit cell parameters, radiographic and pycnometric tellurite densities were determined. $HoSrTeO_{4.5}$: a = 14.50; b = 14.05; c = 9.04Å; $\rho_{roent.}$ = 3.73; $\rho_{pycn.}$ = 3.59 ± 0.04 g/cm^3; $HoBaTeO_{4.5}$: a = 12.10; b = 5.49; c = 11.49Å; $\rho_{roent.}$ = 4.07; $\rho_{pycn.}$ = 3.93 ± 0.06 g/cm^3. The correctness of the results of indexing radiographs of tellurites is confirmed by the good agreement between the experimental and calculated values of the reciprocal values of the squares of interplanar distances ($10^4/d^2$) and the consistency of the values of X-ray and pycnometric densities. It has been established that holmium tellurites are synthesized in monoclinic syngony and have a perovskite-like structure. Quantum-chemical calculations of the stable geometry of the synthesized tellurites were carried out using the Gaussian-2009 software package with the help of the UFF molecular method. In this case, equilibrium internuclear distances (long bonds) and bond angles are the parameters. Based on the results of quantum chemical calculations, models of the geometric structure of new holmium tellurites are presented.

Keywords: double holmium tellurites, X-ray phase analysis, syngony, lattice parameters, quantum chemical calculations, structure models.

Introduction

For a long time, the crystal chemistry of the phases of tellurium-containing oxides has been of interest to many scientists. This interest is caused, on the one hand, by the heterogeneity of the compounds based on the stereochemical activity of the lone electron pair of Te^{IV}, on the other hand, on this basis, assumptions related to the use of tellurites as new pyroelectric and nonlinear optical materials are caused.

Both tellurium dioxide (TeO_2) and selenium (SeO_2) dioxide are widely used in the synthesis of many new solid-state materials due to their lower melting point and triple points (733 for TeO_2, 340 for SeO_2), respectively. These available temperatures allowed them to be used for crystal growth [1]. In addition, the excellent reactivity of TeO_2 and SeO_2 allowed them to be used in the formation of many new oxide materials. Variable coordination media of the Te^{4+} and Se^{4+} cations are also of particular interest. In particular, they demonstrate many structural motives, such as the trigonal pyramid and the square pyramid. If various coordination geometries are combined with other multi-faceted fragments, a greater flexibility of the architecture of the structure is possible. Finally, Te^{4+} and Se^{4+} cations, by their nature, have an asymmetric structural geometry related to an unbound electron pair.

Non-centrosymmetric (NCS) materials are of current and technological interest due to their generation of the second harmonic (SHG), piezoelectric, ferroelectric, and pyroelectric properties [2–5]. With oxide

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materials, structures (NCS) are often observed in materials that contain second-order Jan-Teller distorting cations, octahedral coordinated d^0 transition metal ions (Ti^{4+}, V^{5+}, W^{6+}, etc.) and single pairs of cations (Se^{4+}, Te^{4+}, I^{5+} etc.) [1].

In accordance with these postulates, new double and triple tellurites of a number of *s*-, *d*- and *f*-elements have been synthesized as promising substances with multifunctional properties and their X-ray, thermodynamic and electrophysical properties have been studied at the Department of Inorganic and Technical Chemistry of Buketov Karaganda State University [6–9]. Research in this direction continues.

The aim of this work is the synthesis, X-ray and quantum-chemical studies of new phases of double tellurites of the composition $HoMe^{II}TeO_{4.5}$ (Me^{II} — Sr, Ba).

Experimental

Solid-phase synthesis of compounds was carried out by the method of ceramic technology from holmium (III) oxides of the reagent grade, tellurium (IV) and carbonates of strontium and barium of the analytical grade. Pre-dehydrated at 40 ºC stoichiometric amounts of precursors were thoroughly mixed, ground in an agate mortar. Then, they were annealed in alundum crucibles in the SNOL furnace first at 800 ºC for 20 hours, with periodic grinding in a mortar, then at 1200 ºC for 23 hours, then the mixtures were cooled, mixed, and thoroughly triturated. Low-temperature annealing of the compositions was carried out at a temperature of 400 ºC also for 20 hours.

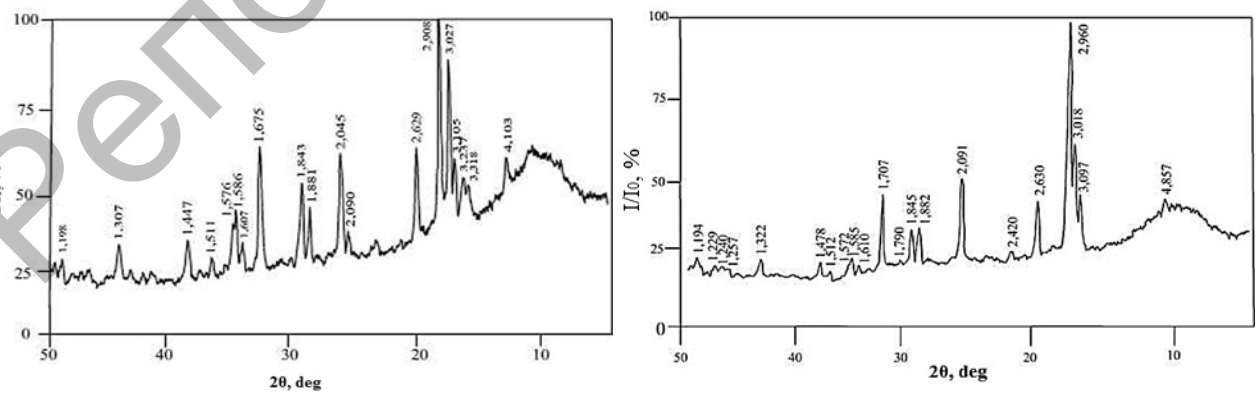
X-ray diffraction investigations of the new phases synthesized were carried out on a DRON-2.0 diffractometer (CuKα-radiation, Ni-filter, $U = 30$ kV, $I = 10$ mA, counter rotation velocity 2 rpm, scale range 1000 imp/s, $\tau = 5$ s, $2\theta = 10–90^{o}$). The intensity of the diffraction peaks was estimated on a 100-point scale. The radiographs of the obtained compounds were indexed by the homology method [10].

The improvement of the computational technologies of modern quantum chemistry led to the creation of powerful commercial software products by individual companies, among which the company Gaussian (USA) founded by John A. Pople stands out. The program «Gaussian-2009» is the latest development from the Gaussian product series. This package of modeling electronic structures is used for developments in the field of chemistry and biochemistry, physics, and other developing fields related to chemical processes [11]. Quantum-chemical calculations of the stable geometry of the synthesized tellurites were carried out using the Gaussian-09 software package with the help of the UFF molecular mechanics method.

Results and Discussion

Each crystalline substance is characterized by its lattice, a certain chemical composition and a certain distribution of atoms in the unit cell of the lattice. The lattice geometry determines the set of interplanar distances (consequently, the Bragg angles θ during diffraction at a given radiation). The individuality and distribution of atoms determines the intensity of the diffracted rays. Qualitative X-ray phase analysis consists in the identification of crystalline phases on the basis of their inherent interplanar spacing $d_{(hkl)}$ values and the corresponding intensities of the $I_{(hkl)}$ lines of the x-ray spectrum.

Figure 1 shows radiographs of the holmium double tellurites synthesized.



a) $HoSrTeO_{4.5}$ *b*) $HoBaTeO_{4.5}$

Figure 1. Radiographs of the holmium double tellurites synthesized

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The results of the X-ray indexing of the holmium tellurites synthesized are shown in Table 1.

Table 1

The results of indexing radiographs of holmium double tellurites

I/I_0, %	d, Å.	$10^4/d^2_{exp.}$	hkl	$10^4/d^2_{calc.}$
$HoSrTeO_{4.5}$				
11	4.770	439	3 0 0	439
13	4.075	602	1 0 2	602
16	3.924	649	2 3 0	650
23	3.070	1061	4 1 1	1061
56	3.015	1100	1 0 –3	1100
100	2.813	1264	0 5 0	1264
31	2.774	1299	3 2 2	1300
10	2.625	1451	3 4 1	1452
35	2.429	1695	4 2 2	1694
20	2.357	1800	4 2 –3	1801
28	2.266	1947	0 6 1	1946
41	2.227	2016	2 6 0	2016
10	2.081	2309	3 6 –1	2308
21	2.030	2426	1 6 2	2424
17	2.025	2439	5 3 2	2440
7	1.958	2607	0 7 1	2604
14	1.873	2851	2 7 1	2852
14	1.830	2987	7 3 –2	2987
7	1.784	3144	0 0 5	3141
$HoBaTeO_{4.5}$				
6	4.857	424	2 0 1	424
24	3.097	1043	0 1 3	1042
48	3.018	1098	4 0 –1	1097
100	2.960	1141	3 1 1	1142
24	2.630	1446	1 2 –1	1446
5	2.420	1708	5 0 –1	1708
37	2.091	2287	2 1 –5	2287
16	1.882	2823	6 0 1	2824
17	1.845	2938	3 0 –6	2938
4	1.790	3121	5 2 –2	3120
34	1.707	3432	1 3 2	3433
5	1.610	3858	1 3 3	3858
9	1.585	3981	5 1 4	3981
5	1.572	4047	5 1 –6	4046
5	1.478	4578	2 0 7	4577
11	1.322	5722	8 2 –1	5722
11	1.257	6329	8 1 3	6328
4	1.248	6421	3 0 8	6421
5	1.223	6686	8 2 2	6686
5	1.194	7014	3 3 6	7014

Based on the X-ray indexing of the synthesized tellurites, it has been established that they crystallize in a monoclinic syngony (Table 2). The correctness of the results of indexing radiographs of tellurites is confirmed by the good agreement between the experimental and calculated values of the reciprocal values of the squares of interplanar distances ($10^4/d^2$) (Table 1), the consistency of the values of X-ray and pycnometric densities (Table 2). In addition, the type of syngony and the unit cell parameters of the compounds are also presented in Table 2.

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Table 2

Syngony type and lattice parameters of HoSrTeO4.5 and HoBaTeO4.5

Compound	Syngony	Lattice parameters, Å			V^0, Å^3	Z	Density, g/cm^3	
		a	b	c			$\rho_{roent.}$	$P_{pycn.}$
$HoSrTeO_{4.5}$	monoclinic	14.50	14.05	9.04	1816.16	10	3.73	3.59±0.04
$HoBaTeO_{4.5}$	monoclinic	12.10	5.49	11.49	747.30	4	4.07	3.93±0.06

The X-ray data show that the tellurites synthesized crystallize in the distorted perovskite structural type P_m3_m. Therefore, it can be assumed that these compounds can possess valuable electrophysical properties [12]. The results of quantum chemical calculations of the geometry of the structure of holmium double tellurites are presented in Table 3.

Table 3

Basic geometric data of holmium double tellurites according to quantum chemical calculations

Bond	*d*, Å	Bond angle	ω, degree
$HoSrTeO_{4.5}$			
O (1) – Te (2)	2.033	Te (3) – O (1) – Te (2)	108
Te (3) – O (1)	2.033	O (4) – Te (3) – O (1)	112
O (5) – Te (2)	2.025	O (6) – Te (3) – O (1)	112
O (7) – Te (2)	2.024	O (5) – Te (2) – O (1)	112
O (4) – Te (3)	2.025	O (7) – Te (2) – O (1)	112
O (6) – Te (3)	2.024	Sr (15) – O (7) – Te (2)	104
Sr (15) – O (7)	2.533	Sr (14) – O (5) – Te (2)	105
Sr (14) – O (5)	2.533	O (8) – Te (2) – O (1)	107
O (9) – Te (3)	2.024	O (9) – Te (3) – O (1)	107
O (8) – Te (2)	2.024	Ho (12) – O (9) – Te (3)	104
Ho (12) – O (9)	2.211	Ho (13) – O (8) – Te(2)	104
Ho (13) – O (8)	2.211	O (11) – Ho (12) – O (9)	180
O (10) – Ho (13)	1.975	O (10) – Ho (13) – O(8)	180
O (11) – Ho (12)	1.975		
$HoBaTeO_{4.5}$			
O (1) – Te (2)	2.003	Te (3) – O (1) – Te (2)	100
Te (3) – O (1)	2.012	O (4) – Te (3) – O (1)	107
O (5) – Te (2)	2.032	O (6) – Te (3) – O (1)	107
O (7) – Te (2)	2.032	O (5) – Te (2) – O (1)	106
O (4) – Te (3)	2.010	O (7) – Te (2) – O (1)	106
O (6) – Te (3)	2.010	Ba (15) – O (7) – Te (2)	107
Ba (15) – O (7)	2.773	Ba (14) – O (5) – Te (2)	107
Ba (14) – O (5)	2.773	O (8) – Te (2) – O (1)	109
O (9) – Te (3)	2.025	O (9) – Te (3) – O (1)	75
O (8) – Te (2)	2.024	Ho (12) – O (9) – Te (3)	105
Ho (12) – O (9)	2.212	Ho (13) – O (8) – Te(2)	104
Ho (13) – O (8)	2.211	O (11) – Ho (12) – O (9)	180
O (10) – Ho (13)	1.975	O (10) – Ho (13) – O(8)	180
O (11) – Ho (12)	1.975		

Based on the results of quantum chemical calculations, models of the structure of new double tellurites are presented. The spatial geometry of the studied compounds of the tellurium composition $HoMTe_{4.5}$ (M is Sr or Ba) is shown in Figure 2.

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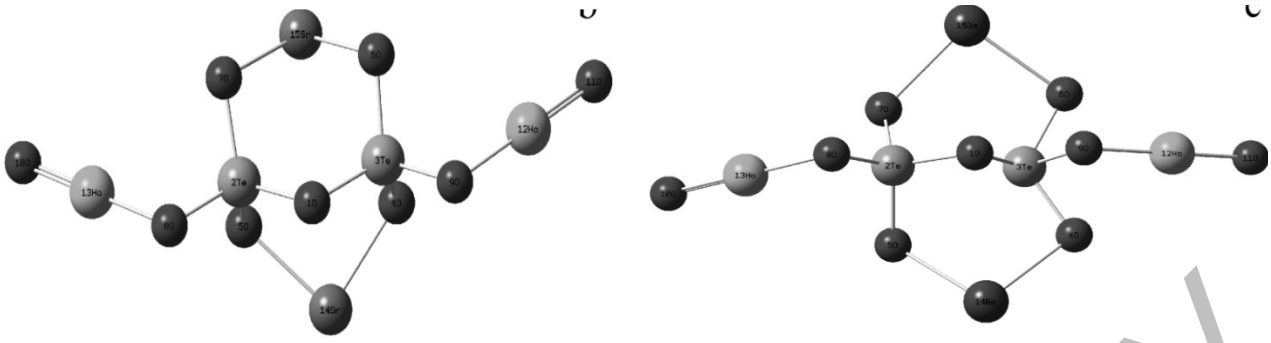

a) $HoSrTeO_{4.5}$ *b*) $HoBaTeO_{4.5}$

Figure 2. Models of the geometric structure of the holmium tellurites synthesized

Conclusion

In the work, new double tellurites of holmium-strontium HoSrTeO4.5 and holmium-barium HoBaTeO4.5 were synthesized using the ceramic technology method. The X-ray phase analysis method was the first to investigate the crystal characteristics of metal-mixed tellurites and to determine the type of syngony, the unit cell parameters, X-ray and pycnometric densities. It has been established that tellurites crystallize in a monoclinic syngony and have a perovskite-like structure. This suggests that these compounds may have unique electrophysical properties.

Based on quantum chemical calculations, models of the geometrical structure of the synthesized tellurites have been proposed. The X-ray characteristics of the holmium tellurite can be the initial information files of fundamental reference books and data banks and are of interest for chemical informatics.

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Гольмий қос теллуриттерін синтездеу, рентгенографиялық және квантты-химиялық зерттеу

Керамикалық технология әдісімен 800–1200 ºС аралығында Ho(II), Te(IV) оксидтері және $SrCO_3$, $BaCO_3$ карбонаттарынан күрделі оксидтік фазалар — $HoMe^{II}TeO_{4,5}$ (Me^{II} — Sr, Ba) құрамды гольмийдің жаңа қос теллуриттері синтезделді. Алғаш рет теллуриттердің құрылысы рентгендік фазалық талдау әдісімен зерттелді. Рентгенфазалық талдау ДРОН-2,0 аппаратында жүргізілді. Дифракциялық максимумдардың қарқындылығы жүз балдық шкаламен бағаланды. Синтезделген ұнтақтардың рентгенограммаларын индицирлеу гомология әдісімен жүргізілді. Теллуриттердің сингония типі, элементар ұяшық параметрлері, ренгенографиялық және пикнометрлік тығыздықтарының мәндері анықталды: $HoSrTeO_{4,5}$: a = 14,50; b = 14,05; c = 9,04Å; $\rho_{рент.}$ = 3,73; $\rho_{пикн.}$ = 3,59 ± 0,04 г/см^3; $HoBaTeO_{4,5}$; a = 12.10; b = 5.49; c = 11.49Å; $\rho_{рент.}$ = 4.07; $\rho_{пикн.}$ = 3.93 ± 0.06 г/см^3. Теллуриттердің рентгенограммаларын индицирлеу нәтижелерінің дұрыстығын жазықтықаралық қашықтықтың квадраттарының кері шамасының ($10^4/d^2$) тәжірибелік және теориялық мәндері мен рентгенографиялық және пикнометрлік тығыздықтарының мәндерінің сәйкестігі дәлелденді. Гольмийдің синтезделген қос теллуриттері моноклиндік сингонияда кристалданатыны және перовскит тәрізді құрылысты екендігі анықталды. Синтезделген теллуриттердің тұрақты геометриясын квантты-химиялық есептеу Gaussian–2009 бағдарламалық пакеті көмегімен, UFF молекулалық механика әдісімен жүргізілді. Бұл жағдайда тепе-теңдік ядроаралық қашықтықтары (байланыс ұзындықтары) және валенттік бұрыштары параметрлері болып табылады. Квантты-химиялық есептеулердің нәтижесінде гольмийдің жаңа қос теллуриттерінің геометриялық құрылыс модельдері ұсынылды.

Кілт сөздер: гольмий қос теллуриттері, рентгенфазалық талдау, сингония, тор параметрлері, квантты-химиялық есептеулер, құрылыс модельдері.

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Синтез, рентгенографическое и квантово-химическое исследования двойных теллуритов гольмия

Методом керамической технологии из оксидов Ho(II), Te(IV) и карбонатов $SrCO_3$, $BaCO_3$ в интервале 800–1200 ºС синтезированы сложные оксидные фазы — новые двойные теллуриты гольмия состава $HoMe^{II}TeO_{4,5}$ (где Me^{II} – Sr, Ba). Методом рентгенофазового анализа впервые исследованы структуры теллуритов. Рентгенофазовый анализ проведен на установке ДРОН-2,0. Интенсивность дифракционных максимумов оценивали по стабильной шкале. Рентгенограммы синтезированных порошков индицированы методом гомологии. Определены тип сингонии, параметры элементарной ячейки, рентгенографические и пикнометрические плотности теллуритов. $HoSrTeO_{4,5}$: a = 14,50; $в$ = 14,05; c = 9,04Å; $\rho_{рент.}$ = 3,73; $\rho_{пикн.}$ = 3,59 ± 0,04 г/см^3; $HoBaTeO_{4,5}$: a = 12,10; в = 5,49; с = 11,49Å; $\rho_{рент.}$ = 4,07; $\rho_{пикн.}$ = 3,93 ± 0,06 г/см^3. Корректность результатов индицирования рентгенограмм теллуритов подтверждается хорошим соответствием экспериментальных и расчетных значений обратных величин квадратов межплоскостных расстояний ($10^4/d^2$) и согласованностью величин рентгеновской и пикнометрической плотностей. Установлено, что синтезированные двойные теллуриты гольмия кристаллизуются в моноклинной сингонии и имеют перовскитоподобную структуру. Квантово-химические расчеты устойчивой геометрии синтезированных теллуритов были проведены с помощью программного пакета Gaussian–2009, методом молекулярной UFF. В данном случае параметрами являются равновесные межъядерные расстояния (длины связей) и валентные углы. На основании результатов квантово-химических расчетов представлены модели геометрического строения новых двойных теллуритов гольмия.

Ключевые слова: двойные теллуриты гольмия, рентгенофазовый анализ, сингония, параметры решетки, квантово-химические расчеты, модели строения.

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