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Thermodynamic properties of pentalead tris(vanadate) chloride

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ABSTRACT

In the present work the temperature dependences of pentalead tris(vanadate) chloride heat capacity have been measured for the first time in the range from 7 to 350 K. The experimental data were used to calculate standard thermodynamic functions, namely the heat capacity $C_p{}^\circ(T)$, enthalpy $H^\circ(T)-H^\circ(0)$, entropy $S^\circ(T)-S^\circ(0)$ and Gibbs function $G^\circ(T)-H^\circ(0)$, for the range from $T\to 0$ to 350 K. The differential scanning calorimetry in temperature interval 298–1473 K was applied to measure temperatures of phase transition and melting of compound under study. The high-temperature X-ray diffraction in range 298–1073 K was used for the determining thermal expansion coefficients.

1. Introduction

Pentalead tris(vanadate) chloride $Pb_5(VO_4)_3Cl$ belongs to structural class of apatite. These compounds have the general formula $M^{II}{}_5(A^VO_4)_3L$ (M^{II} = Ca, Sr, Ba, Cd, Pb; A^V = P, As, V, Mn, Cr; L = OH, F, Cl, Br, I) and can be used as matrix for radioactive wastes ($Pb_5(VO_4)_3I$) [1], bioactive ceramics ($Ca_5(PO_4)_3OH$, $Ca_5(PO_4)_3F$) [2], inorganic pigments ($Ba_5(MnO_4)_3Cl$) [3]. In particular synthetic analogue of mineral vanadinite $Pb_5(VO_4)_3Cl$ is the general source of vanadium. In spite of that there are a few articles consecrated to study of this compound [4,5]. In the present work we have described thermodynamics properties of pentalead tris(vanadate) chloride, which can be used in calculating of solution behavior of vanadate-ion.

2. Experimental

2.1. Sample

Sample of $Pb_5(VO_4)_3Cl$ was prepared by the solid-state reaction between lead vanadate and lead chlorate. The synthesis was performed in a porcelain crucible, into which the reaction mixture with the atomic ration 5Pb + 3V + 1Cl was loaded. The mixture was calcined at 573 and 873 K for 10 h with dispersion in an agate mortar every 2 h. To prove the atomic ration 5Pb + 3V + 1Cl the obtained sample was analyzed on a energo-dispersive roentgen fluorescent spectrometer. The X-ray data and estimated impurity content (0.5–1 wt.%) in the substances led us to conclude that the studied sample was an individual crystalline compound.

2.2. Apparatus and measurement procedure

Shimadzu energo-dispersive roentgen fluorescent spectrometer EDX-900HS (from $_{11}$Na to $_{92}$U) with sensitive detector without liquid nitrogen was used to prove the atomic ration in compound under study.

To measure the heat capacity $C_p{}^\circ$ of the tested substance in the range from 7 to 370 K a BKT-3.0 automatic precision adiabatic vacuum calorimeter with discrete heating was used. The calorimeter design and the operation procedure were described earlier [6,7]. The calorimeter was tested by measuring the heat capacity of high purity copper and reference samples of synthetic corundum and K-2 benzoic acid. The analysis of the results showed that measurement error of the heat capacity of the substance at helium temperature was within ±2% ($5 < T < 20$ K), then it decreased to ±0.5% as the temperature was rising to 40 K, and was equal to ±0.2% at $T > 40$ K.

Thermal experiments were carried out on a LABSYS Setaram differential scanning calorimeter with a heating rate of 10 K/min.

The phase individuality of synthesized compounds was monitored by X-ray diffraction. X-ray diffraction patterns were recorded on a XRD-6000 Shimadzu diffractometer (Cu K_α radiation, geometry θ–2θ) in the 2θ range from 10° to 120° with scan increment of 0.02°.

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High-temperature X-ray diffraction experiments in the range from 298 to 1173 K were carried out on the same diffractometer with increments of 0.02° ranging from 10° to 60° using an HA-1001 Shimadzu attachment.

The experimental thermochemical data set was obtained using a modified Skuratov calorimeter. For the description and details of the experiment, see [8].

3. Results and discussion

3.1. Reaction calorimetry

Calorimetric experiments were carried out in order to calculate standard enthalpies of formation. For this purpose, we chose the thermochemical scheme below where 3 M nitric acid served as a solvent. Mass of the sample was 0.1 g, volume of the solvent was 40 ml. Each of the solution reactions was measured three-five times and error bounds were calculated using Student's distribution.

$$Pb_3(VO_4)_2\,(cr) + HNO_3\,(sln) \rightarrow \text{Solution 1} \qquad (1)$$

$$Pb(NO_3)_2\,(cr) + \text{Solution 1} \rightarrow \text{Solution 2} \qquad (2)$$

$$KCl\,(cr) + \text{Solution 2} \rightarrow \text{Solution 3} \qquad (3)$$

$$Pb_5(VO_4)_3Cl\,(cr) + HNO_3\,(sln) \rightarrow \text{Solution 4} \qquad (4)$$

$$KNO_3\,(cr) + \text{Solution 4} \rightarrow \text{Solution 5} \qquad (5)$$

$$1.5{\cdot}Pb_3(VO_4)_2\,(cr) + 0.5{\cdot}Pb(NO_3)_2\,(cr) + KCl\,(cr) \rightarrow Pb_5(VO_4)_3Cl\,(cr) + KNO_3\,(cr) \qquad (6)$$

$$\begin{aligned}\ln C_p^\circ(T) = {} & A + B\cdot\ln\left(\frac{T}{30}\right) + C\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^2 + D\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^3 + E\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^4 + F\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^5 \\ & + G\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^6 + H\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^7 + I\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^8 + J\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^9 + K\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^{10} + L\cdot\left\{\ln\left(\frac{T}{30}\right)\right\}^{11}\end{aligned} \qquad (8)$$

$$\begin{aligned}C_p^\circ(T) = {} & A + B\cdot\left(\frac{T}{30}\right) + C\cdot\left(\frac{T}{30}\right)^2 + D\cdot\left(\frac{T}{30}\right)^3 + E\cdot\left(\frac{T}{30}\right)^4 + F\cdot\left(\frac{T}{30}\right)^5 + G\cdot\left(\frac{T}{30}\right)^6 + H\cdot\left(\frac{T}{30}\right)^7 \\ & + I\cdot\left(\frac{T}{30}\right)^8 + J\cdot\left(\frac{T}{30}\right)^9 + K\cdot\left(\frac{T}{30}\right)^{10} + L\cdot\left(\frac{T}{30}\right)^{11}\end{aligned} \qquad (9)$$

$$\Delta_r H_1^\circ = -30.6 \pm 0.3;\ \Delta_r H_2^\circ = 4.7 \pm 0.1;\ \Delta_r H_3^\circ = 6.4 \pm 0.3;$$
$$\Delta_r H_4^\circ = -110.8 \pm 0.5;\ \Delta_r H_5^\circ = 9.7 \pm 0.1\ \text{kJ/mol}$$

Reagent ratios were chosen so that the compositions of solutions 3 and 5 were identical. In view of this, the algebraic sum of equations (1.5 × (1) + 0.5 × (2) + (3) – (4) – (5)) leads to Eq. (6):

$$\Delta_r H_6^\circ = 1.5\cdot\Delta_r H_1^\circ + 0.5\cdot\Delta_r H_2^\circ + \Delta_r H_3^\circ - \Delta_r H_{4(4')}^\circ - \Delta_r H_5^\circ;$$
$$\Delta_r H_6^\circ = 64.0 \pm 0.7\ \text{kJ/mol}$$

On the other hand, according to the Hess law,

$$\begin{aligned}\Delta_f H^\circ(298, Pb_5(VO_4)_3Cl, cr) = {} & \Delta_r H_6^\circ(298) + 1.5\cdot\Delta_f H^\circ(298, Pb_3(VO_4)_2, cr) \\ & + 0.5\cdot\Delta_f H^\circ(298, Pb(NO_3)_2, cr) + \Delta_f H^\circ(298, KCl, cr) \\ & - \Delta_f H^\circ(298, KNO_3, cr)\end{aligned} \qquad (7)$$

These equations, together with the enthalpies of reaction (6) and the standard enthalpies of formation of the reagents ($Pb_3(VO_4)_2$ (−2376.5 ± 10.0), $Pb(NO_3)_2$ (−451.7 ± 1.2), KCl (−436.6 ± 0.3), KNO_3 (−494.5 ± 0.5) (kJ/mol) [9]), were used to calculate the standard enthalpies of formation of $Pb_5(VO_4)_3Cl$ at 298.15 K.

$$\Delta_f H^\circ(298,\ Pb_5(VO_4)_3Cl,\ cr) = -3669 \pm 15\ \text{kJ/mol}$$

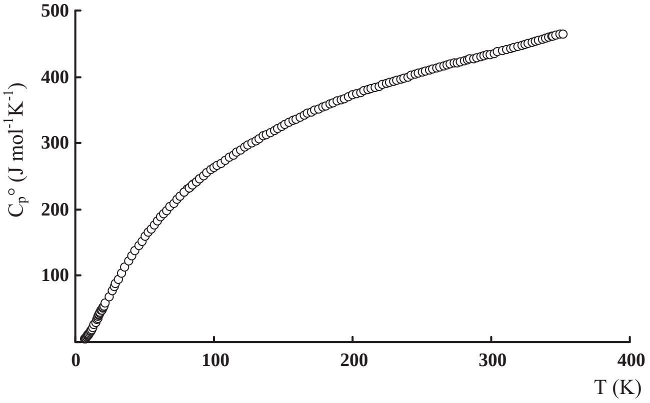

Fig. 1. Temperature dependences of heat capacity of $Pb_5(VO_4)_3Cl$.

3.2. Heat capacity

The C_p° measurements were carried out between 7 and 370 K. The mass of the sample loaded in the calorimetric ampoule of the BKT-3.0 calorimeter was 1.8215 g. There was obtained 171 experimental C_p° values in two series of experiments. The heat capacity of the sample varied from 30% to 70% of the total heat capacity of calorimetric ampoule + substance over the range between 7 and 370 K. The experimental points of C_p° in the temperature interval between T = (7 and 370) K were fitted by means of the least-squares method and polynomial equations (Eqs. (8) and (9)) of the C_p° vs. temperature have been obtained. The corresponding coefficients (A, B, C, etc.) are given in Table S2.

Their root mean square deviation from the averaging $C_p^\circ = f(T)$ curve was 0.15% in the range T = (6–30) K, ±0.075% from T = (25–150) K, ±0.15% between T = (130 and 370) K.

The experimental values of the molar heat capacity of $Pb_5(VO_4)_3Cl$ over the range from 7 to 370 K and the averaging $C_p^\circ = f(T)$ plot are presented in Fig. 1 and Table S1. The heat capacity C_p° of this substance gradually increases with rising temperature and does not show any peculiarities until 350 K.

3.3. Standard thermodynamic functions

To calculate the standard thermodynamic functions (Table 1) of pentalead tris(vanadate) chloride, its C_p° values were extrapolated from the starting temperature of the measurement beginning at approximately 7–0 K by Debye's function of heat capacity:

$$C_p^\circ = nD\left(\frac{\theta_D}{T}\right), \qquad (10)$$

where D is the symbol of Debye's function, $n = 3$ and $\theta_D(Pb_5(VO_4)_3Cl) = 74$ K are specially selected parameters. Eq. (10) with the above parameters describes the experimental C_p° values of the compound between 7 and 13 K with the error of ±1.67%.

In calculating the functions it was assumed that Eq. (10) reproduces the C_p° values of $Pb_5(VO_4)_3Cl$ at $T < 7$ K with the same error.

Table 1
Thermodynamic functions of crystalline $Pb_5(VO_4)_3Cl$; $M(Pb_5(VO_4)_3Cl) = 1416.2703\ g\ mol^{-1}$, $p^\circ = 0.1$ MPa.

T (K)	$C_p{}^\circ(T)$ (J K^{-1} mol^{-1})	$H^\circ(T) - H^\circ(0)$ (kJ mol^{-1})	$S^\circ(T)$ (J K^{-1} mol^{-1})	$-[G^\circ(T) - H^\circ(0)]$ (kJ mol^{-1})
0	0	0	0	0
5	1.807	0.0023	0.6028	0.000754
10	12.74	0.034	4.562	0.01166
15	31.64	0.1425	13.11	0.05415
20	51.92	0.3525	25.05	0.1485
25	71.69	0.6612	38.74	0.3073
30	91.55	1.069	53.56	0.5377
35	110.5	1.575	69.12	0.8444
40	127.3	2.171	85.01	1.230
45	142.9	2.846	100.9	1.695
50	157.8	3.598	116.7	2.239
60	184.4	5.313	147.9	3.563
70	208.0	7.277	178.2	5.194
80	229.3	9.467	207.4	7.123
90	246.6	11.85	235.4	9.338
100	262.6	14.39	262.2	11.83
110	277.2	17.09	287.9	14.58
120	290.8	19.93	312.6	17.58
130	303.6	22.91	336.4	20.83
140	315.7	26.00	359.4	24.31
150	326.9	29.22	381.5	28.01
160	337.1	32.54	403.0	31.94
170	346.7	35.96	423.7	36.07
180	355.7	39.47	443.8	40.41
190	364.3	43.07	463.2	44.94
200	372.4	46.76	482.1	49.67
210	379.8	50.52	500.5	54.58
220	386.8	54.35	518.3	59.68
230	393.5	58.25	535.7	64.95
240	400.2	62.22	552.5	70.39
250	406.7	66.25	569.0	76.00
260	412.9	70.35	585.1	81.77
270	418.7	74.51	600.8	87.70
273.15	420.4	75.83	605.6	89.60
280	424.1	78.73	616.1	93.78
290	429.4	82.99	631.1	100.0
298.15	433.7	86.51	643.0	105.2
300	434.8	87.31	645.7	106.4
310	440.5	91.69	660.1	112.9
320	446.5	96.12	674.1	119.6
330	452.8	100.6	688.0	126.4
340	458.9	105.2	701.6	133.4
350	464.0	109.8	715.0	140.4

The calculations of $H^\circ(T) - H^\circ(0)$ and $S^\circ(T) - S^\circ(0)$ were made by the numerical integration of $C_p{}^\circ = f(T)$ and $C_p{}^\circ = f(\ln T)$ curves, respectively, and the Gibbs function $G^\circ(T) - H^\circ(0)$ was estimated from the enthalpies and entropies at the corresponding temperatures [10]. It was suggested that the error of the function values was ±1% at $T < 40$ K, ±0.5% between 40 and 80 K, ±0.2% in the range from 80 to 350 K.

The absolute entropies of $Pb_5(VO_4)_3Cl$ (Table 1) and the corresponding simple substances Pb (cr), V (cr), O_2 (g) and Cl_2 (g) [9] were used to calculate the standard entropy of formation of the compound under study at 298.15 K, $\Delta_f S^\circ(298.15, Pb_5(VO_4)_3Cl, cr) = -1109.5 \pm 1.9\ J\ K^{-1}\ mol^{-1}$.

Received values of standard enthalpies and entropies of formation were used to calculate the standard Gibbs function of formation $Pb_5(VO_4)_3Cl$ at 298 K by Gibbs–Helmholtz equation $\Delta_f G^\circ(298) = -3338 \pm 16\ kJ\ mol^{-1}$.

Gibbs function temperature dependence of $Pb_5(VO_4)_3Cl$ synthetic reactions (11)–(13) was calculated to analyze thermodynamics of apatite synthetic reaction.

a. lead oxide (II)

$$4.5\,PbO\,(cr) + 1.5\,V_2O_5\,(cr) + 0.5\,PbCl_2\,(cr) \rightarrow Pb_5(VO_4)_3Cl\,(cr) \quad (11)$$

b. lead nitrate

$$4.5Pb(NO_3)_2\,(cr) + 1.5\,V_2O_5\,(cr) + 0.5PbCl_2\,(cr) \rightarrow Pb_5(VO_4)_3Cl\,(cr) + 4.5NO_2\,(g) + 6.75O_2\,(g) \quad (12)$$

c. lead carbonate

$$4.5PbCO_3\,(cr) + 1.5V_2O_5\,(cr) + 0.5PbCl_2\,(cr) \rightarrow Pb_5(VO_4)_3Cl\,(cr) + 4.5CO_2\,(g) \quad (13)$$

Thermodynamics functions of reactions (11)–(13) were calculated by the following equations.

In accordance with the Hess law enthalpies of reactions at $T = 298.15$ K were calculating using standard enthalpies of formation of appropriate reagents at the same temperature:

$$\Delta_r H^\circ(298) = \sum_j \nu_j\, \Delta_f H^\circ(298, j) - \sum_i \nu_i\, \Delta_f H^\circ(298, i),$$

where j relates to reaction products, i relates to reagents.

Reaction entropies at $T = 298.15$ K were calculated using absolute entropies of reagents at the same temperature:

$$\Delta_r S^\circ(298) = \sum_j \nu_j S^\circ(298, j) - \sum_i \nu_i S^\circ(298, i)$$

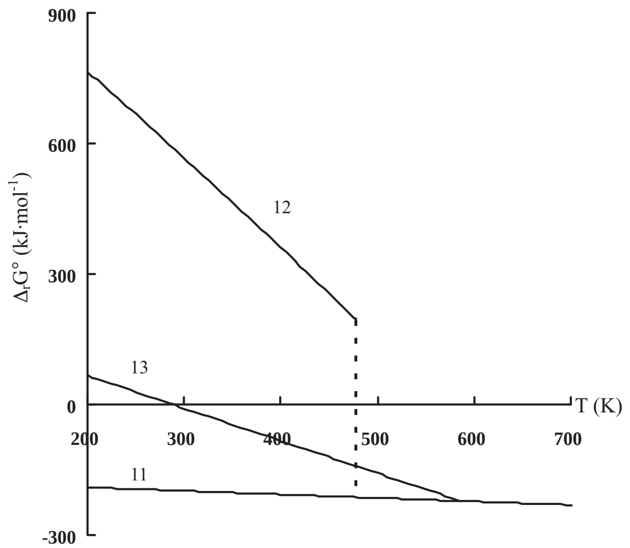

Fig. 2. Plot of Gibbs functions of reactions (11)–(13) vs. temperature for $Pb_5(VO_4)_3Cl$.

Gibbs functions of synthetic reactions at $T = 298.15$ K were computed in concordance with Gibbs–Helmholtz equation:

$$\Delta_rG°(298) = \Delta_rH°(298) - 298.15 \cdot \Delta_rS°(298)$$

In view of the fact that lead nitrate and carbonate decompose at 478 and 588 K respectively solid-state synthetic reactions (12) and (13) lead to reaction (11) (Fig. 2). Temperature of equal probability is the temperature at which Gibbs function of reaction changes sign. Reaction is allowed in thermodynamics if the temperature is higher than temperature of equal probability. It can be calculated only for reaction (13). Gibbs function of the reaction (13) changes according to the following equation:

$$\Delta_rG^\circ_{13} = (-0.755 \cdot T + 218.83)\,\text{kJ/mol} \tag{14}$$

Taking into account Eq. (14) the temperature at which reaction (13) is thermodynamic lawful was calculated: $T = 290 \pm 1$ K. It is remarkable that synthetic reaction (12) is not thermodynamic lawful to the point of decomposition of lead nitrate, while reaction (11) is always proceeds spontaneously.

3.4. Differential scanning calorimetry

Joint application of the high-temperature X-ray diffraction and thermal analysis (TG–DTA) made it possible to establish some peculiarities of processes taking place in the compounds under investigation during heating. Fig. 3 represents DTA curves of $Pb_5(VO_4)_3Cl$, where we can see two endothermic effects at 1031 ($\Delta_{tr}H° = 1.45 \pm 0.05$ kJ mol^{-1}) and 1280 K ($\Delta_mH° = 29.4 \pm 0.9$ kJ mol^{-1}). It was not observed any mass changes on TG curve during experiment, so we can draw a conclusion that the stoichiometric composition of system did not change. The first effect is connected with reversible polymorphic transition "hexagonal" → "monoclinic" with change of crystal system, which can be confirmed by X-ray diffraction data. The second effect is connected with incongruent melting. After the second effect parent phase was not detected. Melting products, found out by XRD analysis, were not identified due to complexity their compositions and lack in PDF 4 and FindIt XRD databases.

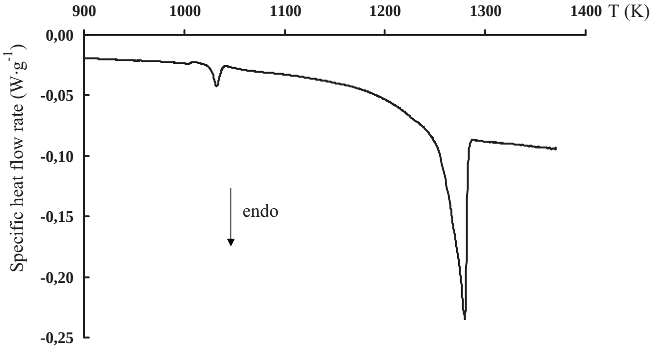

Fig. 3. Plot of the DTA-signal against temperature for $Pb_5(VO_4)_3Cl$.

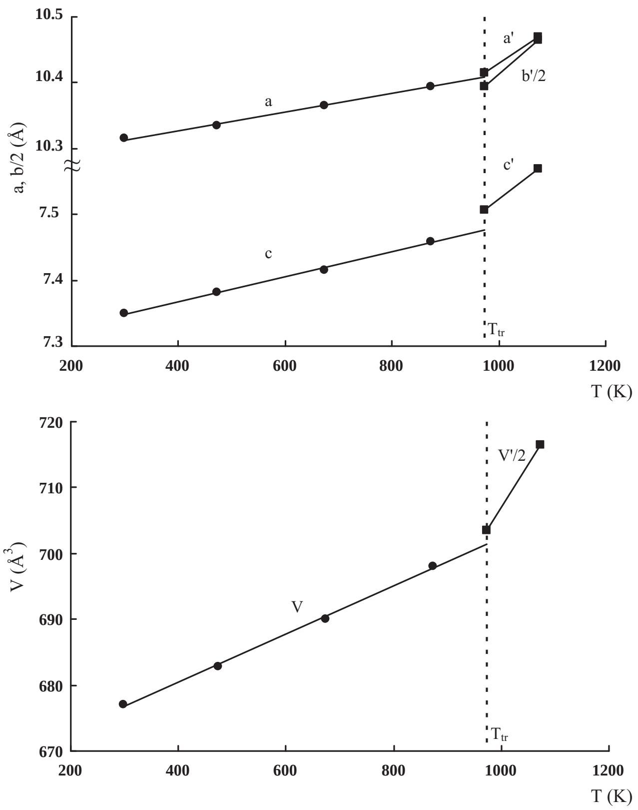

Fig. 4. Unit cell parameters and unit cell volume vs. temperature for $Pb_5(VO_4)_3Cl$.

3.5. High-temperature X-ray diffraction

We carried out high-temperature X-ray diffraction experiments to elucidate structural alterations accompanying the transition. We found that the polymorphic transition lowers the unit cell symmetry from hexagonal (space group $P6_3/m$) to monoclinic (space group $P112_1/b$). At T_{tr}, there is a discontinuity on the unit cell parameter and unit cell volume plots (Fig. 4).

High-temperature X-ray diffraction was used not only for studying phase transitions, but also for determining thermal expansion coefficients (Table 2). For solving this problem, $a = f(T)$ equations were fitted by linear functions and calculations were carried out in KTP program [11].

The data compiled in Table 2 show that $Pb_5(VO_4)_3Cl$ crystals, regardless of the polymorph, have a marked anisotropy of thermal expansion, and this phase of the apatite family may be classified as a strongly expanding compound in terms of the classification system described in [12].

Volume thermal expansion coefficients of monoclinic modifications phase under study in field of polymorphic transition increase fourfold in comparison with similar coefficients of hexagonal modifications.

Table 2
Thermal expansion coefficients vs. temperature for hexagonal and monoclinic modifications of $Pb_5(VO_4)_3Cl$.

T, K	a, Å	$\alpha_a \times 10^6$, K^{-1}	b, Å	$\alpha_b \times 10^6$, K^{-1}	c, Å	$\alpha_c \times 10^6$, K^{-1}	γ,°	$\alpha_\gamma \times 10^6$, K^{-1}	V, Å	$\alpha_V \times 10^6$, K^{-1}	D, kg m^{-3}
298	10.315(1)	13.6	–	–	7.349(1)	18.6	–	–	677.1(1)	45.9	6944
473	10.335(2)		–	–	7.382(1)		–	–	682.9(2)		6885
673	10.366(1)		–	–	7.415(1)		–	–	690.0(2)		6815
873	10.395(1)		–	–	7.459(1)		–	–	698.1(2)		6735
973	10.415(7)	52.8	20.79(1)	67.1	7.507(3)	83.5	120.08(4)	15.0	1407(1)	185.0	6684
1073	10.47(1)		20.93(2)		7.57(4)		120.26(7)		1433(2)		6562

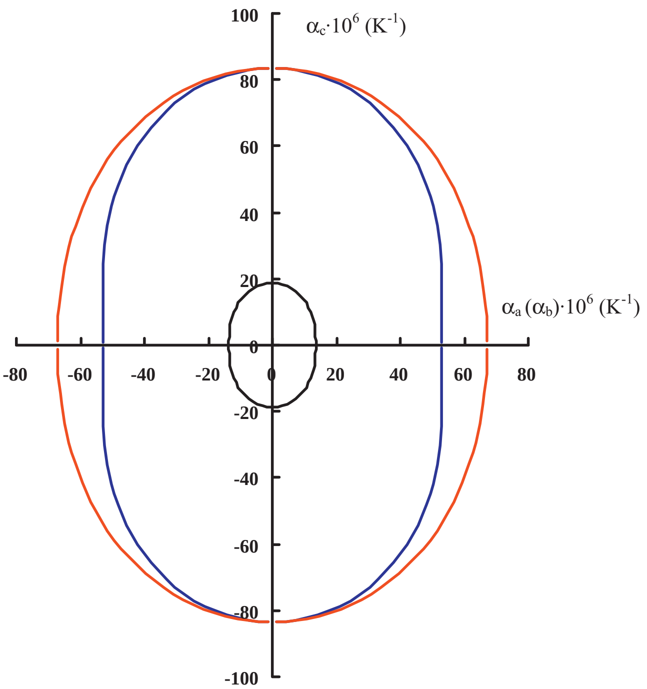

Fig. 5. Thermal expansion diagrams for $Pb_5(VO_4)_3Cl$ at crystallographic plane *ac* for hexagonal modification (black line) and at crystallographic plane *ac* (blue line) and *bc* (red line) for monoclinic modification. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

It is significant that monoclinic modification is pseudo-hexagonal and polymorphic transition can be described as collapse transition in terms of Burgers classification [13]. Also that this transition is reversible. Crystallographic axes *c* are equivalent in both polymorphic modifications. Thereof that $\gamma \neq 120°$ crystallographic axes *a* and *b* of monoclinic modification some differ from crystallographic axes in hexagonal modification (Fig. 6).

Fig. 5 shows thermal expansion diagrams for both modifications of $Pb_5(VO_4)_3Cl$. Value of thermal expansion coefficient in given direction corresponds to length of radius-vector which is traced from origin of coordinates to edge of figure of expansion. In spite of structural alterations, the preferred crystallographic direction upon expansion is the unit cell parameter *c*, which is due to the greater strength of chemical bonds in layers formed by VO_4 tetrahedra compared to interlayer interactions (Fig. 7) [14].

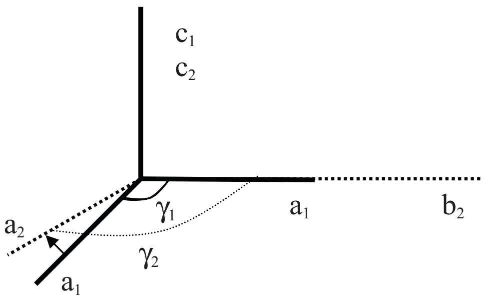

Fig. 6. Change from a hexagonal (subscript 1) to a monoclinic (subscript 2) unit cell upon the polymorphic transformation of vanadinite.

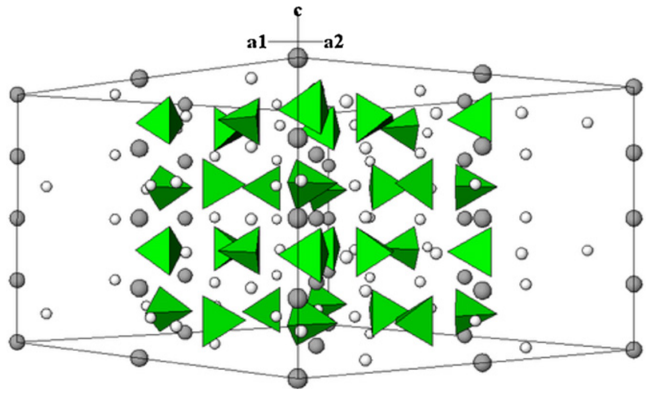

Fig. 7. Schematic of the crystal structure of $Pb_5(VO_4)_3Cl$ (white spheres are Cl atoms, grey spheres – Pb atoms).

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.tca.2010.12.026.

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