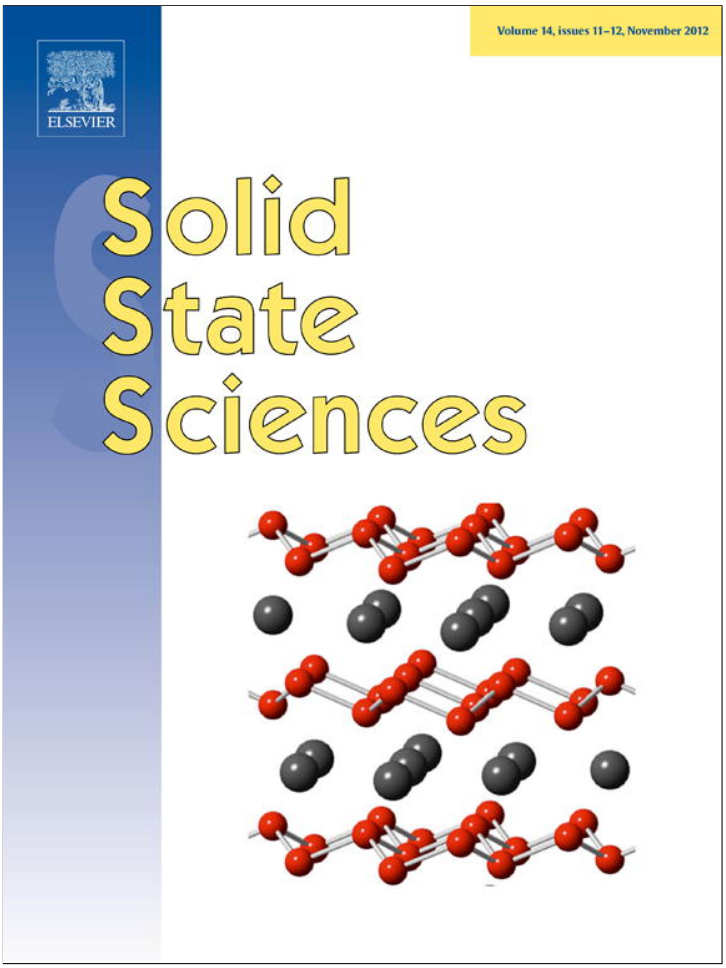

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# Improvement of the method to search low-melting solvents for the crystals $MBaNa(BO_3)_2$ (M = Sc,Y) growth

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ABSTRACT

Matrix interrelation of subsystems coordinates in M–Ba–Na–B–O (M = Sc,Y) system with the compound $MBANa(BO_3)_2$ are derived. Imitation of quaternary eutectic points search by a set of one-dimensional tetrahedron sections (nonplanar tie-lines method) is performed in system $(KCl)_2$–$R_1$–$R_2$-$(LiBO_2)_2$ ($R_1$ = $LiKWO_4$, $R_2$ = $LiKSO_4$), which separates the pentatops $(KCl)_2$-$K_2SO_4$–$R_1$–$R_2$–$(LiBO_2)_2$ and $(KCl)_2$-$(LiBO_2)_2$–$R_1$–$R_2$–$Li_2WO_4$ of system Li,K||Cl,$SO_4$,$WO_4$,$BO_2$. Triangulation of systems A,B,C||X,Y with binary compounds by new algorithms has been considered.



## 1. Introduction

Till now a so-called tie-line method (for the multicomponent eutectic composition determination) was used only as a planar one [1–3], when tetrahedron's sections belong to the planes, which are parallel to tetrahedron faces. Elaboration of theoretical tasks, associated with the transformation of concentration coordinates of multicomponent systems and their subsystems [4], permits to use the set of isopleths, which situate arbitrarily. Efficiency of this approach will be demonstrated in subsystem KCl–$R_1$–$R_2$–$LiBO_2$ with binary compounds $R_1$ = $LiKWO_4$, $R_2$ = $LiKSO_4$. Matrix transformation of mass-centric coordinates is shown by the data for systems M–Ba–Na–B–O (M = Sc,Y) and Li,K||Cl,$SO_4$,$WO_4$,$BO_2$. One more problem of reciprocal salt systems investigation is connected with the polyhedration of multidimensional complexes [5–7]. In this paper new ideas have been offered to triangulate the concentration complexes of A,B||X,Y,Z or A,B,C||X,Y reciprocal systems. Experimental data for the borate systems were taken from [8–10]. Investigation was carried out by means of computer models for phase diagrams [11,12].

## 2. Transformation of coordinates in systems M–Ba–Na–B–O (M = Sc,Y) and Li,K||Cl,$SO_4$,$WO_4$,$BO_2$

System M–Ba–Na–B–O (M = Sc,Y) involves the compounds BaO(0; 1/2; 0; 0; 1/2), $B_2O_3$ (0; 0; 0; 2/5; 3/5), $Na_2O$ (0; 0; 2/3; 0; 1/3), $M_2O_3$(2/5; 0; 0; 0; 3/5), $MBO_3$ (1/5; 0; 0; 1/5; 3/5), $NaBO_2$ (0; 0; 1/4; 1/4; 2/4), $BaNaBO_3$ (0; 1/6; 1/6; 1/6; 3/6), $MBaNa(BO_3)_2$ (1/11; 1/11; 1/11; 2/11; 6/11). The subsystems $MBO_3$–BaO–$B_2O_3$–$Na_2O$, $M_2O_3$–BaO–$B_2O_3$–$Na_2O$ и $MBO_3$–$BaNaBO_3$–$NaBaO_2$ (Fig. 1) [8,9] are considered at the matching of solvents for crystals growth. Let's calculate the coordinates of compound $MBaNa(BO_3)_2$ in subsystems $MBO_3$–BaO–$Na_2O$–$B_2O_3$, $M_2O_3$–BaO–$Na_2O$-$B_2O_3$ and $MBO_3$–$BaNaBO_3$–$NaBO_2$ using the matrix expression $r = M \cdot x$, where $r$ is the column vector of compound $MBaNa(BO_3)_2$ coordinates in pentatop, is the matrix of points coordinates in simplex tops, ч is the column vector of unknowns. The coordinates of tetrahedron $MBO_3$–BaO–$Na_2O$–$B_2O_3$ can be calculated using the matrix expression:

$$\begin{pmatrix} 1/11 \\ 1/11 \\ 1/11 \\ 2/11 \\ 6/11 \end{pmatrix} = \begin{pmatrix} 1/5 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 2/3 & 0 \\ 1/5 & 0 & 0 & 2/5 \\ 3/5 & 1/2 & 1/3 & 3/5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \rightarrow \begin{matrix} x_1 = 0.45 \\ x_2 = 0.18 \\ x_3 = 0.14 \\ x_4 = 0.23 \end{matrix}.$$

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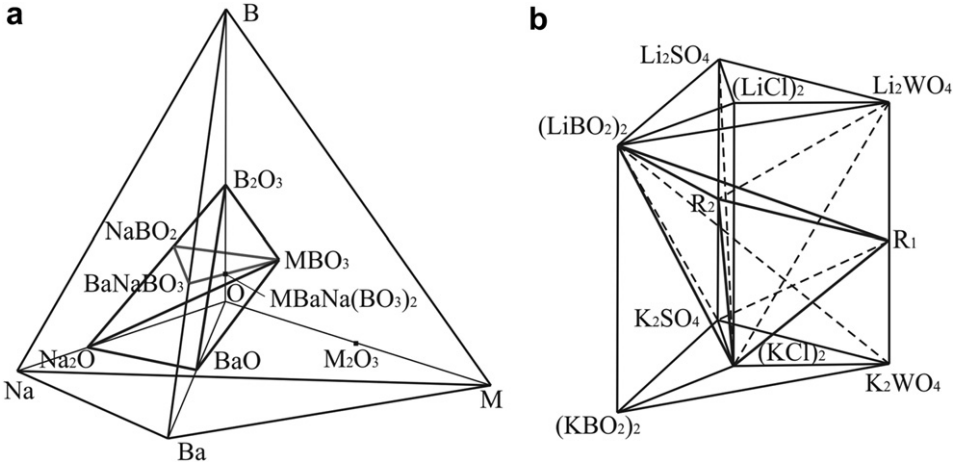


**Fig. 1.** Coordinates transformation in systems M–Ba–Na–B–O ($M$ = Sc,Y) (a) and Li,K||$BO_2$,$SO_4$,$WO_4$,Cl (b).

In similar way the coordinates of compound $MBaNa(BO_3)_2$ in tetrahedron $M_2O_3$–BaO–$Na_2O$–$B_2O_3$ and triangle $MBO_3$–$BaNaBO_3$–$NaBO_2$ are found:

$$\begin{pmatrix} 1/11 \\ 1/11 \\ 1/11 \\ 2/11 \\ 6/11 \end{pmatrix} = \begin{pmatrix} 2/5 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & 2/5 \\ 3/5 & 1/2 & 1/3 & 3/5 \end{pmatrix} \times \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \rightarrow \begin{matrix} x_1 = 0.23 \\ x_2 = 0.18 \\ x_3 = 0.14 \\ x_4 = 0.45 \end{matrix}, \quad \begin{pmatrix} 1/11 \\ 1/11 \\ 1/11 \\ 2/11 \\ 6/11 \end{pmatrix}$$

$$= \begin{pmatrix} 1/5 & 0 & 0 \\ 0 & 1/6 & 0 \\ 0 & 1/6 & 1/4 \\ 1/5 & 1/6 & 1/4 \\ 3/5 & 3/6 & 2/4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \rightarrow \begin{matrix} x_1 = 0.45 \\ x_2 = 0.55 \\ x_3 = 0.00 \end{matrix}.$$

Since the material points $NaBO_2$, $Na_2O$, $B_2O_3$ also have unit masses as well as the tops of initial pentatop M–Ba–Na–B–O, then the composition of compound $NaBO_2$ divides the segment of binary system $Na_2O$-$B_2O_3$ into ratio 5:3 and has the coordinates(0.625; 0.375). The compound $BaNaBO_3$ situated on triangle BaO–$Na_2O$–$B_2O_3$ has the coordinates (0.334; 0.250; 0.416) and divides its area into ratio 4:3:5.

System Li,K||Cl,$SO_4$,$WO_4$,$BO_2$ includes six pentatops ($(KCl)_2$–$K_2SO_4$–$K_2WO_4$–$(LiBO_2)_2$–$(KBO_2)_2$, $(KCl)_2$–$K_2SO_4$–$K_2WO_4$–$(LiBO_2)_2$–$R_1$, $(KCl)_2$–$K_2SO_4$–$R_1$–$R_2$–$(LiBO_2)_2$, $(KCl)_2$–$(LiBO_2)_2$–$R_1$–$R_2$–$Li_2WO_4$, $(KCl)_2$–$R_2$–$Li_2WO_4$–$(LiBO_2)_2$–LiSO$_4$, $(KCl)_2$–$Li_2SO_4$–$Li_2WO_4$–$(LiBO_2)_2$–$(LiCl)_2$) and five tetrahedrons ($(KCl)_2$–$K_2SO_4$–$K_2WO_4$–$(LiBO_2)_2$, $(KCl)_2$–$K_2SO_4$–$R_1$–$(LiBO_2)_2$, $(KCl)_2$–$R_1$–$R_2$–$(LiBO_2)_2$, $(KCl)_2$–$R_2$–$Li_2WO_4$-$(LiBO_2)_2$, $(KCl)_2$–$Li_2SO_4$–$Li_2WO_4$–$(LiBO_2)_2$) [10]. Let's consider the task of transformation of point G(1/4; 1/4; 1/4; 1/4) coordinates given in tetrahedron $(KCl)_2$–$R_1$–$R_2$–$(LiBO_2)_2$ with unit masses in tops relatively the coordinates of initial system. For this purpose, we write the tetrahedron tops in coordinates Li–K–Cl–S–W–B–O: $(KCl)_2$ (0; 1/2; 1/2; 0; 0; 0; 0), $(LiBO_2)_2$ (1/4; 0; 0; 0; 0; 1/4; 2/4), $R_1$(1/7; 1/7; 0; 0; 1/7; 0; 4/7), $R_2$(1/7; 1/7; 0; 1/7; 0; 0; 4/7). The coordinates of point G in initial system Li–K–Cl–S–W–B–O are calculated as:

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \\ z_5 \\ z_6 \\ z_7 \end{pmatrix} = \begin{pmatrix} 0 & 1/7 & 1/7 & 1/4 \\ 1/2 & 1/7 & 1/7 & 0 \\ 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1/7 & 0 \\ 0 & 1/7 & 0 & 0 \\ 0 & 0 & 0 & 1/4 \\ 0 & 4/7 & 4/7 & 2/4 \end{pmatrix} \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix} \rightarrow \begin{matrix} z_1 = 0.134 \\ z_2 = 0.197 \\ z_3 = 0.125 \\ z_4 = 0.036 \\ z_5 = 0.036 \\ z_6 = 0.062 \\ z_7 = 0.410 \end{matrix}.$$

A computer model can be construct both for all system and for individual subsystems, in this case unit masses are placed in the simplex' tops. Let's consider a model of subsystem $(KCl)_2$–$R_1$–$R_2$–$(LiBO_2)_2$.

## 3. Model of subsystem $(KCl)_2$–$R_1$–$R_2$–$(LiBO_2)_2$

Subsystem $(KCl)_2$–$R_1$–$R_2$–$(LiBO_2)_2$ includes 4 liquidus hypersurfaces $Q_i$, a immiscibility hypersurface i, 27 ruled hypersurfaces ($12Q^r_{IJ}$+$12Q^r_{IJK}$+$3i^r$, where $Q^r_{IJ}$ and $Q^r_{IJK}$ are the hypersurfaces with one- and two-dimensional simplexes, $i_r$ are hypersurfaces with one-dimensional simplex bounding the phase regions with immiscibility melt) and a horizontal hyperplane at the temperature of quaternary eutectic $T_\varepsilon$ (Fig. 2, Table 1) [10].

A kinematical method of hypersurfaces describing is used for the computer model simulation [11,12]. In this case, the coordinates of initial components ($I = R_1$, $R_2$, $(KCl)_2$, $(LiBO_2)_2$), 6 binary eutectics ($e_{IJ}$), 4 ternary eutectics ($E_{1-4}$) and quaternary one ($\varepsilon$) are given as initial data. Take into account the curvatures of binary and monovariant liqudus lines, as well as on the hypersurface. Because the solid-phase solubility is missing, then one or two directing elements (surface or two lines) of ruled surfaces are combined with the hyper-prizm edges and then projected into the tetrahedron tops. The shifting of forming line along to the directing surfaces gives the hypersurfaces. The obtained diagram model can be used for the imitation of tie-lines method to find the invariant point by the construction of vertical sections sets.

## 4. Imitation of tie-lines method

The "traditional" tie-lines method initially assumes the giving of three-dimensional vertical section in the plane of which sets two two-dimensional sections [2,5]. The employment of matrix rations between the coordinate systems of considered one-dimensional tie-lines do not need to construct three-dimensional vertical section, and first two two-dimensional sections may not belong to the same plane.

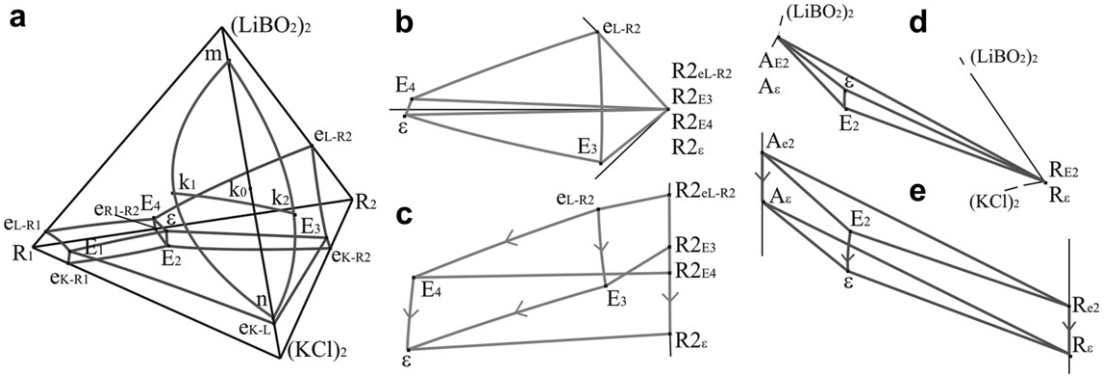


**Fig. 2.** Liquidus and immiscibility hypersurface of subsystem $(KCl)_2$–$R_1$–$R_2$–$(LiBO_2)_2$ (a), ruled hypersurfaces $Q^r_{L\text{-}R2}$ (b–c) and $Q^r_{R1-R2-K}$ (d–e) in XYZ and TXY projections.

**Table 1**
Contour of hypersurfaces ($(KCl)_2 \equiv K$, $(LiBO_2)_2 \equiv L$).

| Symbol | Contour | Symbol | Contour | Symbol | Contour |
|---|---|---|---|---|---|
| $Q_{R1}$ | $R_1 e_{R1-R2} e_{K-R1} e_{L-R1} E_1 E_2 E_4 \varepsilon$ | $Q^r_{R1-K}$ | $E_2 e_{K-R1} E_1 \varepsilon K_\varepsilon K_{E1} K_{E2} K_{eKR1}$ | $Q^r_{K-L-R1}$ | $E_1 \varepsilon K_\varepsilon L_\varepsilon L_{E1} K_{E1}$ |
| $Q_{R2}$ | $R_2 e_{R1-R2} e_{K-R2} e_{L-R2} E_2 E_3 E_4 \varepsilon$ | $Q^r_{R2-K}$ | $E_3 e_{K-R2} E_2 \varepsilon K_\varepsilon K_{E2} K_{E3} K_{eKR2}$ | $Q^r_{R1-R2-K}$ | $E_2 \varepsilon R1_\varepsilon R2_\varepsilon R2_{E2} R1_{E2}$ |
| $Q(KCl)_2$ | $K e_{K-R1} e_{K-R2} e_{K-L} E_1 E_2 E_3 \varepsilon$ | $Q^r_{K\text{-}L}$ | $E_3 e_{K-L} E_1 \varepsilon K_\varepsilon K_{E1} K_{E3} K_{eK-L}$ | $Q^r_{R1\text{-}K\text{-}R2}$ | $E_2 \varepsilon R1_\varepsilon K_\varepsilon K_{E2} R1_{E2}$ |
| $Q(LiBO)_2$ | $L e_{L-R1} e_{L-R2} e_{K-L} E_1 E_3 E_4 \varepsilon mnk_1k_2$ | $Q^r_{R1-L}$ | $E_4 e_{L-R1} E_1 \varepsilon L_\varepsilon L_{E1} L_{E4} L_{eL-R1}$ | $Q^r_{R2-K-R1}$ | $E_2 \varepsilon R2_\varepsilon K_\varepsilon K_{E2} R2_{E2}$ |
| $i$ | $mnk_1k_2k^0$ | $Q^r_{R2\text{-}L}$ | $E_4 e_{L-R2} E_3 \varepsilon L_\varepsilon L_{E3} L_{E4} L_{eL-R2}$ | $Q^r_{R2-K-L}$ | $E_3 \varepsilon R2_\varepsilon K_\varepsilon K_{E3} R2_{E3}$ |
| $Q^r_{R1-R2}$ | $E_4 e_{R1-R2} E_2 \varepsilon R1_\varepsilon R1_{E2} R1_{E4} R1_{eR1R2}$ | $Q^r_{L\text{-}K}$ | $E_3 e_{K-L} E_1 \varepsilon L_\varepsilon L_{E1} L_{E3} L_{eK-L}$ | $Q^r_{R2-L-K}$ | $E_3 \varepsilon R2_\varepsilon L_\varepsilon L_{E3} R2_{E3}$ |
| $Q^r_{K-R1}$ | $E_2 e_{K-R1} E_1 \varepsilon R1_\varepsilon R1_{E1} R1_{E2} R1_{eK-R1}$ | $Q^r_{R1-R2-L}$ | $E_4 \varepsilon R1_\varepsilon R2_\varepsilon R2_{E4} R1_{E4}$ | $Q^r_{K-L-R2}$ | $E_3 \varepsilon K_\varepsilon L_\varepsilon L_{E3} K_{E3}$ |
| $Q^r_{L-R1}$ | $E_4 e_{L-R1} E_1 \varepsilon R1_\varepsilon R1_{E1} R1_{E4} R1_{eL-R1}$ | $Q^r_{R1-L-R2}$ | $E_4 \varepsilon R1_\varepsilon L_\varepsilon L_{E4} R1_{E4}$ | $i^r_{mn}$ | $mnk_1k_2$ |
| $Q^r_{R2-R1}$ | $E_4 e_{R1-R2} E_2 \varepsilon R_2 \varepsilon R2_{E2} R2_{E4} R2_{eR1R2}$ | $Q^r_{R2-L-R1}$ | $E_4 \varepsilon R2_\varepsilon L_\varepsilon L_{E4} R2_{E4}$ | $i^r_m$ | $mk_1k_2L_{m(n)}L_{k1}L_{k2}$ |
| $Q^r_{K-R2}$ | $E_3 e_{K-R2} E_2 \varepsilon R2_\varepsilon R2_{E2} R2_{E3} R2_{eK-R2}$ | $Q^r_{R1-K-L}$ | $E_1 \varepsilon R1_\varepsilon K_\varepsilon K_{E1} R1_{E1}$ | $i^r_n$ | $nk_1k_2L_{m(n)}L_{k1}L_{k2}$ |
| $Q^r_{LR2}$ | $E_4 e_{L-R2} E_3 \varepsilon R2_\varepsilon R2_{E3} R2_{E4} R2_{eLR2}$ | $Q^r_{R1-L-K}$ | $E_1 \varepsilon R1_\varepsilon L_\varepsilon L_{E1} R1_{E1}$ | $H_\varepsilon$ | $R1_\varepsilon R2_\varepsilon K_\varepsilon L_\varepsilon \varepsilon$ |

In the first stage, two-dimensional section is given by two points on the tetrahedron sides within the projection one of liquidus hypersurface. For example, section $s_1$(0.52; 0.45; 0; 0.03)–$s_2$(0.44; 0.48; 0.08; 0) (Fig. 3a) intersects the liquidus hypersurface $Q_{R2}$ (line 1–2), ruled hypersurfaces $Q^r_{R2R1}$ (3–4), $Q^r_{R1R2L}$ (5–6), $Q^r_{R1R2K}$ (6–7), hyperplane at $T_\varepsilon$ (8–6–9) (Fig. 3b). The section point 6≡r belongs to common forming simplex $R_{1\varepsilon}R_{2\varepsilon}\varepsilon$ of ruled hypersurfaces $Q^r_{R1R2L}$ и $Q^r_{R1R2K}$ at $T_\varepsilon$. Taking the segment $s_1s_2$ length equal to unit, we obtain that the section base is divided into the parts with the lengths 0.54 and 0.46 (Fig. 3b) at the projecting of point $r$ on the section base. So the coordinates of point $r$ can be calculated using matrix transformation [4]:

$$\begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix} = \begin{pmatrix} s1_1 & s2_1 \\ s1_2 & s2_2 \\ s1_3 & s2_3 \\ s1_4 & s2_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{pmatrix}$$

$$= \begin{pmatrix} 0.52 & 0.44 \\ 0.45 & 0.48 \\ 0 & 0.08 \\ 0.3 & 0 \end{pmatrix} \begin{pmatrix} 0.54 \\ 0.46 \end{pmatrix} \rightarrow \begin{matrix} r_1 = 0.483, \\ r_2 = 0.464, \\ r_3 = 0.037, \\ r_4 = 0.016. \end{matrix}$$

In the second stage, the section passing through the obtained point r and arbitrary point $s_3$(0.6; 0.4; 0; 0) of tetrahedron edge $R_1R_2$ is constructed to intersection with with tetrahedron side

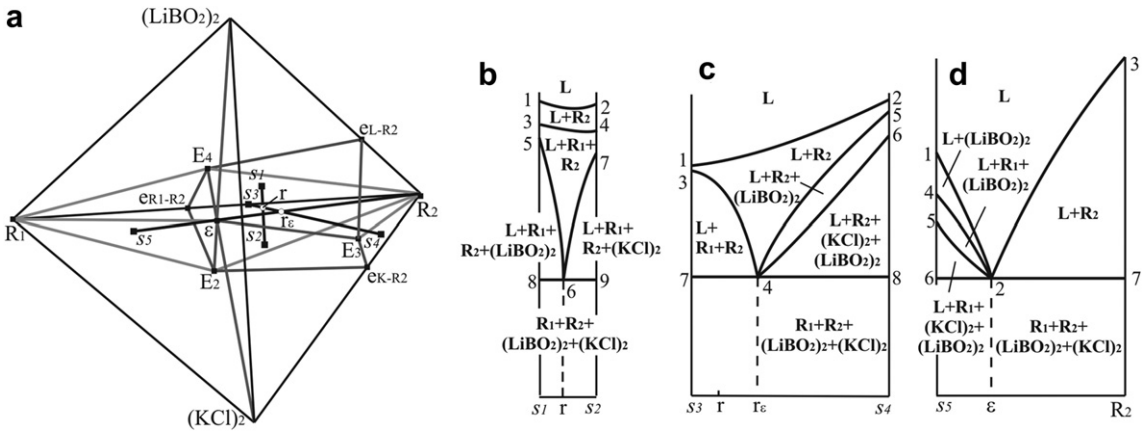


**Fig. 3.** Scheme of arrangement (a) of sections $s_1s_2$ (b), $s_3s_4$ (c), $R_2s_5$ (d).

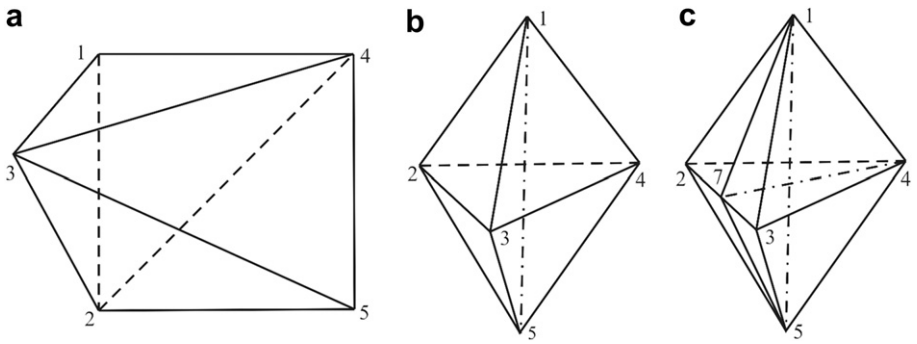


**Fig. 4.** Microcomplex 12345 of ternary reciprocal system (a) and the variants of hexahedron triangulation: alternative of plane 324 and diagonal 15 (b), alternative of diagonals 47 and 15 (c).

$R_2$–$(KCl)_2$–$(LiBO_2)_2$ in point $s_4$ (Fig. 3a). Simultaneously solution of equation of plane $R_2$–$(KCl)_2$–$(LiBO_2)_2$ and segment $s_3$r gives the coordinates of point $s_4$(0; 0.73; 0.19; 0.08). The section $s_3s_4$ intersects the liquidus $Q_{R2}$ (line 1–2), ruled hypersurfaces $Q^r_{R2R1}$ (3–4), $Q^r_{R2L}$ (4–5), $Q^r_{R2LK}$ (4–6) (Fig. 3c) and one-dimensional forming segment $R_{2\varepsilon}\varepsilon$ of ruled hypersurface at the temperature of quaternary eutectic in point $4 \equiv r_\varepsilon$. Then we define that the point $r_\varepsilon$ divides the segment base into the parts with lengths 0.66 and 0.34, and calculate its coordinates:

$$\begin{pmatrix} r_{\varepsilon 1} \\ r_{\varepsilon 2} \\ r_{\varepsilon 3} \\ r_{\varepsilon 4} \end{pmatrix} = \begin{pmatrix} s3_1 & s4_1 \\ s3_2 & s4_2 \\ s3_3 & s4_3 \\ s3_4 & s4_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} r_{\varepsilon 1} \\ r_{\varepsilon 2} \\ r_{\varepsilon 3} \\ r_{\varepsilon 4} \end{pmatrix}$$

$$= \begin{pmatrix} 0.6 & 0 \\ 0.4 & 0.73 \\ 0 & 0.19 \\ 0 & 0.08 \end{pmatrix} \begin{pmatrix} 0.66 \\ 0.34 \end{pmatrix} \rightarrow \begin{matrix} r_{\varepsilon 1} = 0.396, \\ r_{\varepsilon 2} = 0.512, \\ r_{\varepsilon 3} = 0.064, \\ r_{\varepsilon 4} = 0.028. \end{matrix}$$

Next section is construct along to ray $R_2r_\varepsilon$ till the intersection the side $R_1$–$(KCl)_2$–$(LiBO_2)_2$ in point $s_5$ (Fig. 3a). The equations of plane $R_1$–$(KCl)_2$–$(LiBO2)_2$ and segments $R_2r_\varepsilon$ are simultaneously solved for the calculation of point $s_5$ coordinates. Section $R_2s_5$ intersects $Q_L$ (1–2), $Q_K$ (2–3), $Q^r_{LR1}$ (2–4), $Q^r_{R1LK}$ (2–5) and $H_\varepsilon$ (Fig. 3d). Section point 2 is the desired point $\varepsilon$, dividing the section base into the pats with length 0.7 and 0.3. Its coordinates are calculated as:

$$\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{pmatrix} = \begin{pmatrix} A_1 & s5_1 \\ A_2 & s5_2 \\ A_3 & s5_3 \\ A_4 & s5_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0.81 \\ 1 & 0 \\ 0 & 0.13 \\ 0 & 0.06 \end{pmatrix} \begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix} \rightarrow \begin{matrix} \varepsilon_1 = 0.567, \\ \varepsilon_2 = 0.3, \\ \varepsilon_3 = 0.091, \\ \varepsilon_4 = 0.042. \end{matrix}$$

## 5. Variants of hexahedron triangulation

The separation of tetrahedron 3456 in system A,B||X,Y,Z visualized as the prizm 123456 with given triangulation of bounding ternary reciprocal systems by the diagonals 24, 34, 35 produces the microcomplex 12345 (Fig. 4a). Because the diagonal 24 dividing the square 2145 into triangles 214 and 245 is known, then the microcomplex 12345 can be considered as the degenerated hexahedron consisting of tetrahedral 1234 and 2345 with common side 234. It's appropriate to consider and the second variant of triangulation of non-degenerated hexahedron 12345 into three tetrahedrons (1523 + 1534+1524) with three adjacent sides (153, 154, 152) and with common internal edge 15 (Fig. 4b). In these two variants, there are a competition of common side 234 of two tetrahedrons and common edge 15 of tree tetrahedrons. Since second variant of triangulation is not implemented in real physical-chemical systems, we can suggest that the optimal triangulation is determined by the minimal quantity of tetrahedrons. The advent of additional top (chemical compound) 7 on the edge 23 produces that each of two variants of triangulation gives to 4 tetrahedrons: 1347 + 1247+5347 + 5247 or 1527 + 1537+1534 + 1524 (Fig. 4c). In addition, both variant of triangulation with the competing internal diagonals 15 or 47 became equiprobable ones. Real variant should be examined by the experimental check of point of diagonals intersection: $15 \cap 47$.

The triangulation of microcomplex 12345 (Fig. 4a) by Kraeva's method [5] gives only one variant of dividing into two tetrahedrons (1234 и 2345) and does not reveal the internal diagonal, because the matrix of adjustments contents only unit elements. Whereas the employment of algorithm for the hexahedron with additional point 7 on the edge 23 (Fig. 4c) identifies two variants of triangulation. In first case, the diagonal 15 is unit element, and diagonals 23 and 47 are zero ones. And the multiplication of adjustments list gives: $(x_2 + x_3)(x_4 + x_7) = x_2x_4 + x_2x_7 + x_3x_4 + x_3x_7$. After the inversion we obtain four tetrahedrons 1357, 1345, 1257 and 1245. In second case, the matrix and list of adjustments content unit diagonal 47 and zero diagonals 15 and 23. The multiplication of adjustments list $(x_1 + x_5)(x_2 + x_3) = x_1x_2 + x_1x_3 + x_2x_5 + x_3x_7$ and the inversion produce four tetrahedrons 3457, 2457, 1347, 1245.

## 6. Summary

Computer models make possible the convenient visualization of phase diagrams geometrical structure, as well as realize the different variants of their sections. The understanding of phase diagram regularities allows us to predict the view of two-dimensional sections based on their arrangement relative to the liquidus elements, and exclude the possible errors in their graphics. Nonplanar tie-lines method has been developed by means of computer model with the matrix transformation of coordinates for the determination of invariant compositions. The alternative variants of triangulations, realized at the forming of binary compound, are considered as very useful in reciprocal salt systems.

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