Relation between the Mass-Centric Coordinates in Multicomponent Salt Systems

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An algorithm which allows to define relations between concentration coordinates of subsystems formed in the initial system consisting of simple elements is proposed. The same algorithm gives a possibility to determine the conditions under which the point belongs to the given concentration simplex or complex.

Key words: Polyhedration; Concentration Simplex and Complex; Mass-Centric Coordinates.

1. Introduction

Often different concentration coordinates are used for multicomponent systems. Even in binary salt systems like $LnHal_3$-MHal [1 – 3], there is a possibility to visualize them as $LnHal_3$-MHal or $Ln_{1/3}$Hal-MHal. In the former case an $LnHal_3$-$(MHal)_3$ system looks like the same, but it depends on addition of an additional component to form a ternary system. More complex problems appear when different concentration coordinates are used for the subsystem of the same system, especially when their dimensions don't coincide. The ternary oxide compounds of the composition $1:2:11$ obtained in the system La_2O_3-MgO-Al_2O_3 [4] may be used in binary, ternary or more complex systems as $LaMgAl_{11}O_{19}$, $La_2Mg_2Al_{22}O_{38}$ and so on. Hence, it is necessary to estimate possibilities to represent data produced from different sources in one concentration coordinate system.

Investigations of n-component salt systems give answers to many practical questions concerned with different methods to represent salt mixture concentrations:

1) preparation of a binary, ternary, quaternary or any n-component mixture from several mixtures of different compositions;
2) dilution of an initial mixture by adding one or several liquids;
3) determination of relative weight proportions of equilibrium phases or individual structure elements in binary, ternary, quaternary, ..., n-component mixtures at different temperatures;
4) analysis of phase equilibrium in mixtures containing two, three, four, ..., n phases.

As is known, phase equilibrium is visualized in the form of the concentration simplex or complex with m corners within the n-component system. Every simplex $(m \leq n)$ or complex $(m > n)$ makes its own system of concentration coordinates. Physical features of such coordinates are:

a) relations between line lengths, triangle and quadrangle areas, volumes of appropriate three-dimensional figures and so on [5, 6];
b) mass-centric coordinates of subsystems simplexes, expressed in terms of mass or mole fractions, when in the simplexes tops are placed different numbers of moles (integer or fractional);
c) concentrations of reciprocal systems (complexes on the intersections of the n-component simplex with a hyperplane) are expressed by ratios of cations and anions or ions with the same sign.

Nevertheless any n-component system has the initial mass-centric system. Its coordinates correspond to the relative partition of the initial simple elements (atoms)

forming oxides, salts, and other complex compounds in the system.

2. Relations between Mass-Centric Coordinates of Simplexes

Two coordinate systems $Z(Z_1, \ldots, Z_n)$, which expresses the n-component concentration, and $X(X_1, \ldots, X_m)$, representing the mass-centric coordinates of any m-dimensional $(m \le n)$ subsystem, are connected by the concentration matrix **K** of dimension $[n \times m]$ in a form [7]

$$\mathbf{Z} = \mathbf{K} \cdot \mathbf{X} \text{ or}$$

$$\begin{pmatrix} Z_1 \\ \cdots \\ Z_n \end{pmatrix} = \begin{pmatrix} K_{11} \cdots K_{m1} \\ \cdots \cdots \cdots \\ K_{1n} \cdots K_{mn} \end{pmatrix} \begin{pmatrix} X_1 \\ \cdots \\ X_m \end{pmatrix}, \quad (1)$$

where the matrix elements K_{ij} $(i = \overline{1,n}, j = \overline{1,m})$ are **Z**-coordinates of the subsystem **X** corners. The point with the vector-column **Z**-coordinates belongs to the simplex if all elements of the vector **X** satisfy the condition

$$0 \le X_j \le 1. \quad (2)$$

For instance, if the compounds $\mathrm{M} = \mathrm{A_2D}$, $\mathrm{K} = \mathrm{BD_3}$, $\mathrm{N} = \mathrm{AC}$, $\mathrm{L} = \mathrm{A_2BD_4} = \mathrm{A_2D} \cdot \mathrm{BD_3}$ and $\mathrm{P} = \mathrm{A_3BCD_4} = \mathrm{A_2BD_4} \cdot \mathrm{AC} = \mathrm{A_2D} \cdot \mathrm{BD_3} \cdot \mathrm{AC}$ are formed with $n = 4$ in the system A-B-C-D (Fig. 1a), then the **Z**-coordinates of the points are equal to M(2/3, 0, 0, 1/3), K(0, 1/4, 0, 3/4), N(1/2, 0, 1/2, 0), $\mathrm{L} \in \mathrm{MK}$ (2/7, 1/7, 0, 4/7), $\mathrm{P} \in \mathrm{LN} \in \Delta\mathrm{MNK}$ (3/9, 1/9, 1/9, 4/9). Equation (1) helps to recalculate the coordinates of the compounds L and P in the subsystem M-K-N at $m = 3$:

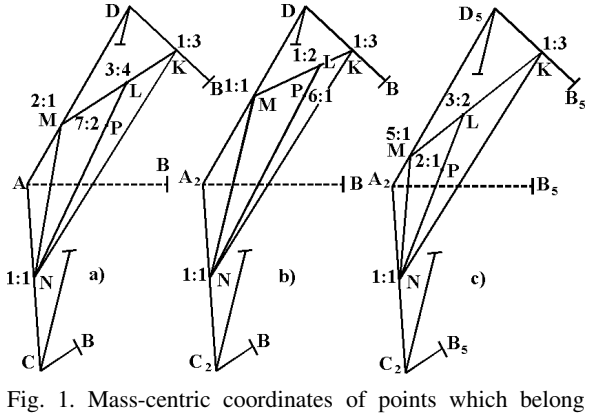

Fig. 1. Mass-centric coordinates of points which belong to the system A-B-C-D and change in dependence on the weight coefficients q_i of the initial components: (a) $q_\mathrm{A} = q_\mathrm{B} = q_\mathrm{C} = q_\mathrm{D} = 1$; (b) $q_\mathrm{A} = q_\mathrm{C} = 2$, $q_\mathrm{B} = q_\mathrm{D} = 1$; (c) $q_\mathrm{A} = q_\mathrm{C} = 2$, $q_\mathrm{B} = q_\mathrm{D} = 5$.

$$\mathrm{L} = \mathrm{A_2D} \cdot \mathrm{BD_3} : \begin{pmatrix} 2/7 \\ 1/7 \\ 0 \\ 4/7 \end{pmatrix} = \overset{\mathrm{A_2D}\ \mathrm{BD_3}}{\begin{pmatrix} 2/3 & 0 \\ 0 & 1/4 \\ 0 & 0 \\ 1/3 & 3/4 \end{pmatrix}} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix},$$

$$X_1 = 3/7, X_2 = 4/7, \mathrm{L} \in \mathrm{MK} \text{ as } 3:4,$$

$$\mathrm{P} = \mathrm{A_2D} \cdot \mathrm{BD_3} \cdot \mathrm{AC} : \begin{pmatrix} 3/9 \\ 1/9 \\ 1/9 \\ 4/9 \end{pmatrix} = \overset{\mathrm{A_2D}\ \mathrm{BD_3}\ \mathrm{AC}}{\begin{pmatrix} 2/3 & 0 & 1/2 \\ 0 & 1/4 & 0 \\ 0 & 0 & 1/2 \\ 1/3 & 3/4 & 0 \end{pmatrix}} \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \end{pmatrix},$$

$$Y_1 = 3/9, Y_2 = 4/9, Y_3 = 2/9, \mathrm{P} \in \Delta\mathrm{MNK} \text{ as } 3:4:2,$$

and of the compound P in the subsystem L-N at $m = 2$:

$$\mathrm{P} = \mathrm{A_2BD_4} \cdot \mathrm{AC} : \begin{pmatrix} 3/9 \\ 1/9 \\ 1/9 \\ 4/9 \end{pmatrix} = \overset{\mathrm{A_2BD_4}\ \mathrm{Ac}}{\begin{pmatrix} 2/7 & 1/2 \\ 1/7 & 0 \\ 0 & 1/2 \\ 4/7 & 0 \end{pmatrix}} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix},$$

$$X_1 = 7/9, X_2 = 2/9, \mathrm{P} \in \mathrm{LN} \text{ as } 7:2.$$

These relations are useful to define whether the compound (and the point that corresponds to it) belongs to some subsystem. It is sufficient to introduce the **Z**-coordinates of this point into the equation of corresponding line or plane. For instance:

$$\mathrm{P} \in \mathrm{LN}, \text{ because } \frac{\mathrm{P}_i - \mathrm{L}_i}{\mathrm{N}_i - \mathrm{L}_i} = \text{const or}$$

$$\frac{3/9 - 2/7}{1/2 - 2/7} = \frac{1/9 - 1/7}{-1/7} = \frac{1/9}{1/2} = \frac{4/9 - 4/7}{-4/7} = 2/9;$$

$$\mathrm{P} \in \Delta\mathrm{MNK}, \text{ because}$$

$$\begin{vmatrix} P_1 - M_1 & P_2 - M_2 & P_3 - M_3 \\ K_1 - M_1 & K_2 - M_2 & K_3 - M_3 \\ N_1 - M_1 & N_2 - M_2 & N_3 - M_3 \end{vmatrix} = \begin{vmatrix} 3/9 - 2/3 & 1/9 & 1/9 \\ -2/3 & 1/4 & 0 \\ 1/2 - 2/3 & 0 & 1/2 \end{vmatrix} = 0.$$

It is possible to place in any corner of the initial system A-B-C-D either a unit mass or the mass produced to some weight coefficient q. Let, for instance, the masses equal to 2 be placed in the corners A and C (Fig. 1b). In such a case the point M on the edge AD moves to its center, and its **Z**-coordinates change to (1/2, 0, 0, 1/2). The coordinates of the points L and P will vary too:

$$\mathrm{L} = (\mathrm{A_2})\mathrm{BD_4} : (1/6, 1/6, 0, 4/6) \text{ and}$$

$$\mathrm{P} = (\mathrm{A_2})_{3/2}(\mathrm{C_2})_{1/2}\mathrm{BD_4} : (3/14, 2/14, 1/14, 8/14),$$

$$\mathrm{L} = (\mathrm{A_2})\mathrm{D}\cdot\mathrm{BD_3}: \begin{pmatrix}1/6\\1/6\\0\\4/6\end{pmatrix} = \overset{\mathrm{A_2D}\ \mathrm{BD_3}}{\begin{pmatrix}1/2 & 0\\0 & 1/4\\0 & 0\\1/2 & 3/4\end{pmatrix}} \begin{pmatrix}X_1\\X_2\end{pmatrix},$$

$$X_1 = 1/3, X_2 = 2/3, \mathrm{L} \in \mathrm{MK} \text{ as } 1:2,$$

$$\mathrm{P} = \begin{matrix}(\mathrm{A_2})\mathrm{D}\\ \cdot\mathrm{BD_3}\cdot(\mathrm{AC})\end{matrix}: \begin{pmatrix}3/14\\2/14\\1/14\\8/14\end{pmatrix} = \overset{(\mathrm{A_2})\mathrm{D}\ \mathrm{BD_3}\ \mathrm{AC}}{\begin{pmatrix}1/2 & 0 & 1/2\\0 & 1/4 & 0\\0 & 0 & 1/2\\1/2 & 3/4 & 0\end{pmatrix}} \begin{pmatrix}Y_1\\Y_2\\Y_3\end{pmatrix},$$

$$Y_1 = 2/7, Y_2 = 4/7, Y_3 = 1/7, \mathrm{P} \in \Delta\mathrm{MNK} \text{ as } 2:4:1,$$

$$\mathrm{P} = (\mathrm{A_2})\mathrm{BD_4}\cdot\mathrm{AC}: \begin{pmatrix}3/14\\2/14\\1/14\\8/14\end{pmatrix} = \overset{(\mathrm{A_2})\mathrm{BD_4}\ \ \mathrm{AC}}{\begin{pmatrix}1/6 & 1/2\\1/6 & 0\\0 & 1/2\\4/6 & 0\end{pmatrix}} \begin{pmatrix}X_1\\X_2\end{pmatrix},$$

$$X_1 = 6/7, X_2 = 1/7, \mathrm{P} \in \mathrm{LN} \text{ as } 6:1.$$

The coordinates of the salts Na_2SO_4, NaF and Na_3FSO_4 formed by the components A = Na, B = S, C = F, D = O will change if one puts half of a mole, 1 mol and so on in the corners of the subsystem Na_2SO_4-NaF [8]. For comparing the experimental data for the systems obtained by different authors it is necessary to present them in the common coordinate system Na-S-F-O and to select the respective weight coefficients. For instance, to express the eutectic coordinates in the subsystem Na_2SO_4-Na_3FSO_4, where one equivalent NaF corresponds to two equivalents Na_2SO_4 in the binary compound Na_3FSO_4 point it is sufficient to find the weight coefficients q_{Na}, q_F, q_S, q_O, for which the point Na_3FSO_4 divides the line Na_2SO_4-NaF in the ratio 2:1. As a result, in such a case the weight coefficients must be equal to $q_{Na} = q_F = 2$ and $q_S = q_O = 5$ (Fig. 1c).

Traditionally the composition of an n-component mixture in a salt system is expressed in reference books by mass (B_i), mole (N_i) or equivalent (E_i) fractions. Mass and mole fractions are linked by the formulas [8]

$$B_i = N_i M_i / \sum_{j=1}^{n} (N_j M_j),$$

$$N_i = B_i / \left[M_i \sum_{j=1}^{n} (B_j / M_j) \right],$$

where M_i is the mass of 1 mol of the i-th component. Relations between equivalent and mole fractions depend on the weight coefficients of q_i the mixture initial elements:

$$N_i = E_i / \left[q_i \sum_{j=1}^{n} (E_j / q_j) \right].$$

3. Concentration Coordinates of Reciprocal Systems (Complexes)

If any cross-section of the system by a (hyper)plane gives a complex, then it is considered as a reciprocal subsystem and the mixture concentration is given by the ratio of salts placed to the complex corners or the ratio of ions with the same signs. For instance, in the ternary reciprocal system B, D // M, N the mixture concentration can be expressed both in terms of the initial salts [BM], [BN], [DM], [DN] or in terms of the ion $b = [\mathrm{b}^+]$, $d = [\mathrm{d}^+]$, $m = [\mathrm{m}^-]$, $n = [\mathrm{n}^-]$ fractions, where

$$b + d = 1, \quad m + n = 1,$$
$$[\mathrm{BM}] + [\mathrm{BN}] + [\mathrm{DM}] + [\mathrm{DN}] = 1.$$

In the first case they are calculated as areas of opposite rectangles (Fig. 2a):

$$\begin{aligned}&[\mathrm{BM}] = b\cdot m, \quad [\mathrm{BN}] = b\cdot n = b\cdot(1-m) \text{ and}\\ &[\mathrm{DM}] = d\cdot m, \quad [\mathrm{DN}] = d\cdot n = d\cdot(1-m),\end{aligned} \tag{3}$$

in the second case inverse relations may be written in the form

$$\begin{aligned}&b = [\mathrm{BM}] + [\mathrm{BN}], \quad d = [\mathrm{DM}] + [\mathrm{DN}],\\ &m = [\mathrm{BM}]/([\mathrm{BM}] + [\mathrm{BN}]),\\ &n = [\mathrm{BN}]/([\mathrm{BM}] + [\mathrm{BN}]).\end{aligned} \tag{4}$$

Sometimes the coordinates are expressed as ratios $[\mathrm{b}^+]/[\mathrm{d}^+] = u$, $[\mathrm{m}^-]/[n^-] = v$. Taking into account $b + d = 1$ and $m + n = 1$, we obtain

$$b = u/(1+u) \text{ and } m = v/(1+v). \tag{5}$$

For instance, the ternary eutectic coordinates in the system Ag, Rb // Cl, NO_3 are represented as: 117°, $[\mathrm{Rb}^+]/[\mathrm{Ag}^+] = 0.43$, $[\mathrm{Cl}^-]/[\mathrm{NO_3}^-] = 0.04$ [9, quoted by 10]. Recalculations with the help of (5) give these data in traditional form:

$$b = 0.301, \quad d = 0.699,$$
$$m = 0.038, \quad n = 0.962 \text{ and}$$
$$[\mathrm{BM}] = 0.011, \quad [\mathrm{BN}] = 0.290,$$
$$[\mathrm{DM}] = 0.027, \quad [\mathrm{DN}] = 0.672.$$

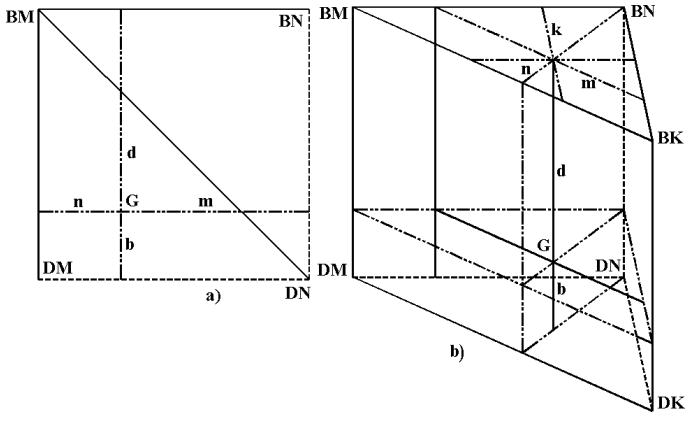

Fig. 2. Relations between the coordinates, represented by ion portions, or relations of initial salts in the reciprocal salt systems: (a) B, D // M, N ($b = 0.25$, $d = 0.75$, $m = 0.6$, $n = 0.4$); (b) B, D // M, N, K ($b = 0.25$, $d = 0.75$, $m = 0.3$, $n = 0.4$, $k = 0.3$).

Since the coordinates n and b are similar to Cartesian coordinates of the point **G**, the coordinates of the reciprocal system B, D // M, N and its subsystem V-W-U can be related by the matrix equation

$$\begin{pmatrix} 1 \\ G_n \\ G_b \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ V_n & W_n & U_n \\ V_b & W_b & U_b \end{pmatrix} \begin{pmatrix} G_1 \\ G_2 \\ G_3 \end{pmatrix},$$

where (V_n, V_b), (W_n, W_b), (U_n, U_b) are Cartesian coordinates of the subsystem corners (units in the upper row of the matrix underline the fact that the G_1, G_2, G_3 coordinates are normalized: $G_1 + G_2 + G_3 = 1$). For instance, at V = BM, W = DN, U = DM the matrix receives the form $\begin{pmatrix} 1\,1\,1 \\ 0\,1\,0 \\ 1\,0\,0 \end{pmatrix}$ and $G_2 = G_n$, $G_3 = G_b$, $G_1 = 1 - G_n - G_b$.

Concentrations in the quaternary reciprocal system B, D // M, N, K are also expressed in two coordinate form, using either the mass portions of the initial salts [BM], [BN], [BK], [DM], [DN], [DK] or the ions [b^+], [d^+], [m^-], [n^-], [k^-]. Both coordinates are normalized:

$$b + d = 1, \quad m + n + k = 1,$$
$$[\mathrm{BM}] + [\mathrm{BN}] + [\mathrm{BK}] + [\mathrm{DM}] + [\mathrm{DN}] + [\mathrm{DK}] = 1.$$

If the concentration is expressed in terms of the initial salt portions then the volumes of oppositely placed figures must be calculated (Fig. 2b):

$$\begin{aligned} &[\mathrm{BM}] = b \cdot m, \quad [\mathrm{BN}] = b \cdot n, \quad [\mathrm{BK}] = b \cdot k, \\ &[\mathrm{DM}] = d \cdot m, \quad [\mathrm{DN}] = d \cdot n, \quad [\mathrm{DK}] = d \cdot k. \end{aligned} \tag{6}$$

The ion method to express concentrations is related with them in the following form:

$$\begin{aligned} b &= [\mathrm{BM}] + [\mathrm{BN}] + [\mathrm{BK}], \\ d &= [\mathrm{DM}] + [\mathrm{DN}] + [\mathrm{DK}], \\ m &= [\mathrm{BM}]/([\mathrm{BM}] + [\mathrm{BN}] + \mathrm{BK}]), \\ n &= [\mathrm{BN}]/([\mathrm{BM}] + [\mathrm{BN}] + [\mathrm{BK}]), \\ k &= [\mathrm{BK}]/([\mathrm{BM}] + [\mathrm{BN}] + [\mathrm{BK}]). \end{aligned} \tag{7}$$

The coordinates of the point **G** of subsystems B // M, N, K and D // M, N, K are the mass-centric ones. As an application, the b coordinate is used for the 3-dimensional mapping point in the concentration prism (Fig. 2b).

4. Determination of Concentration Point Belonging to a Simplex or Complex

Analyzing phase equilibria usually requires solving two tasks (straight and inverse):

1) to determine if a point belongs to the concentration simplex or complex;
2) to choose a point which corresponds to a given chemical interaction.

To solve these tasks (1) is the best means. It is enough to express the point coordinates as concentrations of the initial simple elements in it and to check conditions (2) for the simplex corner coordinates.

If some point **G** belongs to the concentration simplex border then one or more of its coordinates X_j are equal to border values of condition (2). For instance, the concentration of the point **G** corresponding to the interaction $3\mathrm{BM} + 5\mathrm{DN} + 7\mathrm{DK} = 3\mathrm{KCl} + 5\mathrm{CaWO_4} + 7\mathrm{CaMoO_4}$

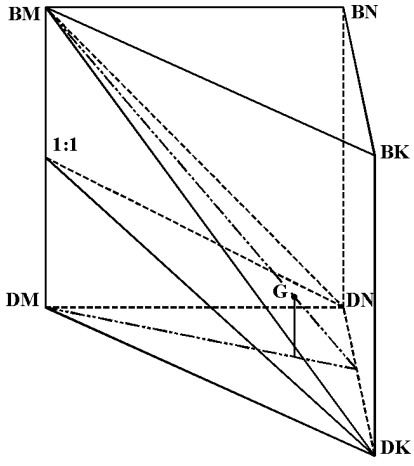

Fig. 3. The point **G** belongs to the subsystem BM-DN-DK = KCl-$CaWO_4$-$CaMoO_4$ of the salt system B, D // M, N, K at B = K, D = Ca, M = Cl, N = WO_4, K = MoO_4.

in the system K, Ca // Cl, WO_4, MoO_4 [11], where B = K, D = Ca, M = Cl, N = WO_4, K = MoO_4, is connected with the subsystem (tetrahedron) $(KCl)_2$-$KCaCl_3$-$CaWO_4$-$CaMoO_4$ (Fig. 3) by the equation

$$\begin{pmatrix} 12/78 \\ 3/78 \\ 3/78 \\ 5/78 \\ 7/78 \\ 48/78 \end{pmatrix} = \begin{pmatrix} 0 & 1/5 & 1/6 & 1/6 \\ 1/2 & 1/5 & 0 & 0 \\ 1/2 & 3/5 & 0 & 0 \\ 1/2 & 3/5 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/6 \\ 0 & 0 & 4/6 & 4/6 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{pmatrix},$$

from which it follows that $X_1 = 6/78$, $X_2 = 0$, $X_3 = 30/78$, $X_4 = 42/78$. The coordinate X_2 is equal to zero and thus the considered point is on the tetrahedron $(KCl)_2$-$KCaCl_3$-$CaWO_4$-$CaMoO_4$ face BM-DN-DK = KCl-$CaWO_4$-$CaMoO_4$.

To define if a point belongs to some concentration complex with m corners $(m > n)$ in the reciprocal system, the ion balance method based on the graph theory has been developed [11]. It is possible to list and to enumerate the corners of every elementary concentration subsystem, which can be formed in the n-component system by the incidences matrix [12, 13].

However, (1) is more preferable in this case too, because any complex can be divided into simplexes or complexes. It is sufficient to solve the equations of type (1) with respect to these simplexes and to verify conditions (2) every time. If conditions (2) are satisfied for one of the simplexes then it means that the point belongs to the considered complex.

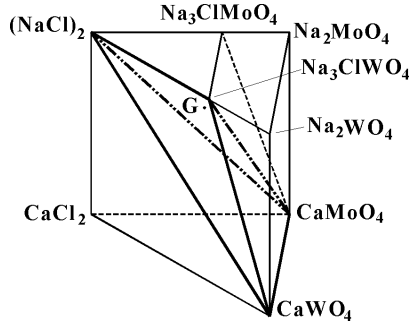

Fig. 4. Subsystems of the reciprocal system Ca, Na // Cl, WO_4, MoO_4: The simplex $CaCl_2$-$(NaCl)_2$-$CaMoO_4$-$CaWO_4$ and the two complexes $CaWO_4$-Na_3ClWO_4-$(NaCl)_2$-Na_3ClMoO_4-$CaMoO_4$, $CaWO_4$-Na_3ClWO_4-Na_3ClMoO_4-$CaMoO_4$, where $Na_3ClMoO_4 = 1\ (2NaCl) : 2Na_2MoO_4$, $Na_3ClWoO_4 = 1\ (2NaCl) : 2Na_2WO_4$.

For instance, the concentration space of the reciprocal system Ca, Na // Cl, WO_4, MoO_4 can be divided into three subsystems: the simplex $CaCl_2$-$(NaCl)_2$-$CaMoO_4$-$CaWO_4$, and two complexes $CaWO_4$-Na_3ClWO_4-$(NaCl)_2$-Na_3ClMoO_4-$CaMoO_4$ and $CaWO_4$-Na_3ClWO_4-Na_3ClMoO_4-$CaMoO_4$ [11] (Fig. 4). To determine which concentration simplex includes the point **G** given by the initial relation of salts

$$5CaCl_2 + 9Na_2MoO_4 + 3CaWO_4 + 13NaCl + 11Na_2WO_4,$$

it is sufficient to write its concentration in the system Ca-Na-Cl-W-Mo-O in not yet normalized units: [Ca] - 8, [Na] - 53, [Cl] - 23, [W] - 14, [Mo] - 9, [O] - 92. The coordinates $Z_1 = 8/199$, $Z_2 = 53/199$, $Z_3 = 23/199$, $Z_4 = 14/199$, $Z_5 = 9/199$, $Z_6 = 92/199$ become elements of the vector **Z** after normalization. If one writes the concentration matrix **K** for the simplex $CaWO_4$-$(NaCl)_2$-$CaMoO_4$-$CaCl_2$ and places to its mass-centric coordinates as columns of four of its corners then the solution of (1)

$$\begin{pmatrix} 8/199 \\ 53/199 \\ 23/199 \\ 14/199 \\ 9/199 \\ 92/199 \end{pmatrix} = \begin{pmatrix} 1/6 & 0 & 1/6 & 1/3 \\ 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 2/3 \\ 1/6 & 0 & 0 & 0 \\ 0 & 0 & 1/6 & 0 \\ 4/6 & 0 & 4/6 & 0 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{pmatrix}$$

gives $X_1 = 84/199$, $X_2 = 106/199$, $X_3 = 54/199$, $X_4 = -45/199 < 0$. If one of the coordinates is negative (X_4) then the corresponding point does not belong to this simplex.

As for the stable complex $CaWO_4$-Na_3ClWO_4-$(NaCl)_2$-Na_3ClMoO_4-$CaMoO_4$, it is necessary to divide it by planes into simplexes and to extend (1) to every simplex. For instance, it turns out that the point **G** belongs to the simplex $CaWO_4$-$(NaCl)_2$-Na_3ClMoO_4-Na_3ClWO_4 within the complex because all **X**-coordinates satisfy condition (2):

$$\begin{pmatrix} 8/199 \\ 53/199 \\ 23/199 \\ 14/199 \\ 9/199 \\ 92/199 \end{pmatrix} = \begin{pmatrix} 1/6 & 0 & 0 & 0 \\ 0 & 1/2 & 3/9 & 3/9 \\ 0 & 1/2 & 1/9 & 1/9 \\ 1/6 & 0 & 0 & 1/9 \\ 0 & 0 & 1/9 & 0 \\ 4/6 & 0 & 4/9 & 0 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{pmatrix}$$

or $X_1 = 48/199$, $X_2 = 16/199$, $X_3 = 81/199$, $X_4 = 54/199$. Hence, the resulting interaction may be described in the form

$$\begin{aligned} &5CaCl_2 + 9Na_2MoO_4 + 3CaWO_4 \\ &+ 13NaCl + 11Na_2WO_4 \\ &= 3CaWO_4 + 11Na_3ClWO_4 + 8NaCl \\ &+ 4Na_3ClMoO_4 + 5CaMoO_4. \end{aligned}$$

5. Conclusions

All different methods to express the n-component mixture concentrations can be represented by only one system of coordinates which corresponds to the input of its simple elements to the mixture composition. This coordinate system allows

1) to correlate concentration coordinates of various subsystems (both simplexes and complexes);
2) to compare experimental data represented in the literature by different concentration coordinates;
3) to analyze some phase reaction possibility by verifying if the concentration point, which corresponds to the given chemical interaction, belongs to some elementary concentration simplex (or complex).

Acknowledgements

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