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Quaternary Reciprocal Systems with the Inner Diagonals: Variants of Polyhedration

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Abstract. New algorithm has been offered to divide a concentration complex of reciprocal system for the subsystems. It is based on the relations between the number of complex polyhedron vertexes and resulting number of simplexes. Method is demonstrated on the quaternary systems**.** It is easy realized in the software, and is very effective in the cases with inner points (compounds) and with the competition of inner diagonals.

Introduction

Usually [1] the adjacency matrix is used for the multicomponent systems polyhedration. As this process is very time-consuming, especially at many additional vertexes (new compounds) of polyhedron, special software has been elaborated [2]. Its input is an adjacency list (formed from the adjacency matrix zero elements) and its output is a list of simplexes. The program [3] defines interrelation between concentration coordinates of subsystems, formed in the initial system and given by chemical elements, and determines condition when the point belongs to the given concentration simplex or complex (at $0<X_i<1$ for all solutions of the matrix equation $Z=MX$, where matrixes Z and M describes the point coordinates and the subsystem vertexes concentration).

Method of A. Zykov, used in graphs theory to design the independent sub-graphs family on the base of the adjacency matrix R and its list R_L [4], may be applied for polyhedration too. A. Kraeva was first [5], who used it for the polyhedrons dividing (with zero elements in the adjacency list R_L). So, the algorithm may be named as the ZK Algorithm (of Zykov-Kraeva).

Polyhedration by the ZK algorithm

The polyhedron with triangulated faces is presented as a non-oriented graph. Its original vertexes and the points of new compounds (on edges, faces and inside it) are numbered. Elements of the adjacency list are zero elements of the adjacency matrix. They are multiplied with regard to the absorption law. The inversion is applying to the multiplication result. And at last the simplexes list is formed. The system K,Ca,Na||NO$_3$,Cl has two binary D_1=KCl·CaCl$_2$, D_2=KNO$_3$·2Ca(NO$_3$)$_2$ and a ternary D_3=KNO$_3$·2Ca(NO$_3$)$_2$·KCl [6] compounds (Fig. 1). Connections NaNO$_3$-D_2, D_2-D_3, KNO$_3$-D_3, Ca(NO$_3$)$_2$-D_3, KCl-D_3, Ca(NO$_3$)$_2$-D_1, NaCl-Ca(NO$_3$)$_2$, NaCl-KNO$_3$, D_1-D_3, D_1-NaCl in bordering systems have been given *a posteriori*. All points are numerated: x_1=KCl, x_2=CaCl$_2$, x_3=NaCl, x_4=KNO$_3$, x_5=Ca(NO$_3$)$_2$, x_6=NaNO$_3$, x_7=D_1, x_8=D_2, x_9=D_3. Two pairs of lines $x_6x_7+x_6x_9$ or $x_3x_8+x_3x_9$ are in competition to be the inner diagonals. If to use the connections x_6x_7 and x_6x_9, then an algorithm outputs only five 3D simplexes (tetrahedrons) and six 2D simplexes (triangles). Hence, these inner diagonals do not satisfy the given triangulation of the prism faces. So, other connections are to be used: x_3x_8=(NaCl)(D_2), x_3x_9=(NaCl)(D_3). After multiplication according to the absorption law $(x_1+x_2x_5x_6x_8)(x_2+x_4x_6x_8x_9)(x_4+x_5x_7)(x_6+x_7x_9)(x_7+x_8)=x_1x_2x_4x_6x_7+x_1x_2x_5x_6x_7+x_2x_5x_6x_7x_8+x_1x_2x_4x_7x_9+x_1x_2x_5x_7x_9+x_1x_2x_4x_6x_8+x_1x_4x_6x_8x_9+x_2x_4x_5x_6x_8$, and inverse of each product, the polyhedration is successfully finished by dividing the initial complex into 8 simplexes: $x_3x_5x_8x_9+x_3x_4x_8x_9+x_1x_3x_4x_9+x_3x_5x_6x_8+x_3x_4x_6x_8+x_3x_5x_7x_9+x_2x_3x_5x_7+x_1x_3x_7x_9$.

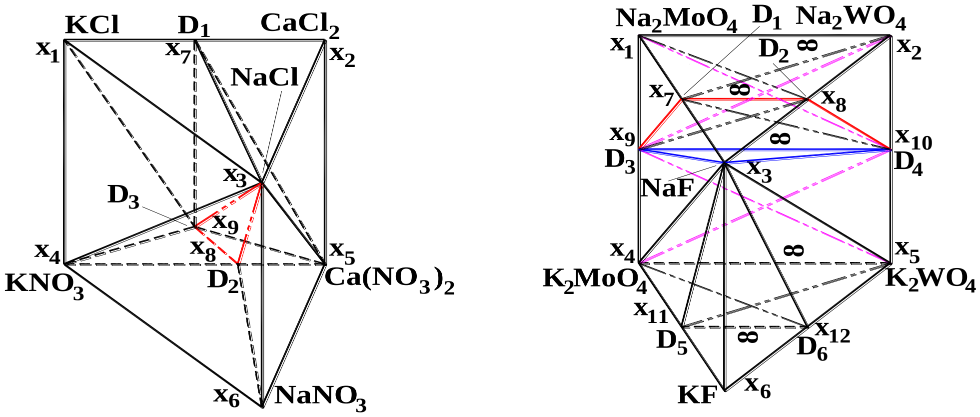

Fig. 1. Polyhedration of the quaternary reciprocal systems: K,Ca,Na||NO$_3$,Cl - with two binary and a ternary compounds; Na,K||MoO$_4$,WO$_4$,F - with solid solutions.

The system Na,K||MoO$_4$,WO$_4$,F (Fig. 1) has incongruent D$_1$=2NaF·Na$_2$MoO$_4$, D$_2$=2NaF·Na$_2$MoO$_4$, D$_3$=Na$_2$MoO$_4$·K$_2$MoO$_4$, D$_4$=Na$_2$WO$_4$·K$_2$WO$_4$ and congruent D$_5$=KF·K$_2$MoO$_4$, D$_6$=KF·K$_2$WO$_4$ compounds. They form micro-complexes $x_1x_2x_7x_8$, $x_1x_2x_9x_{10}$, $x_4x_5x_9x_{10}$, $x_4x_5x_{11}x_{12}$ and $x_7x_8x_9x_{10}$ of solid solutions [1].

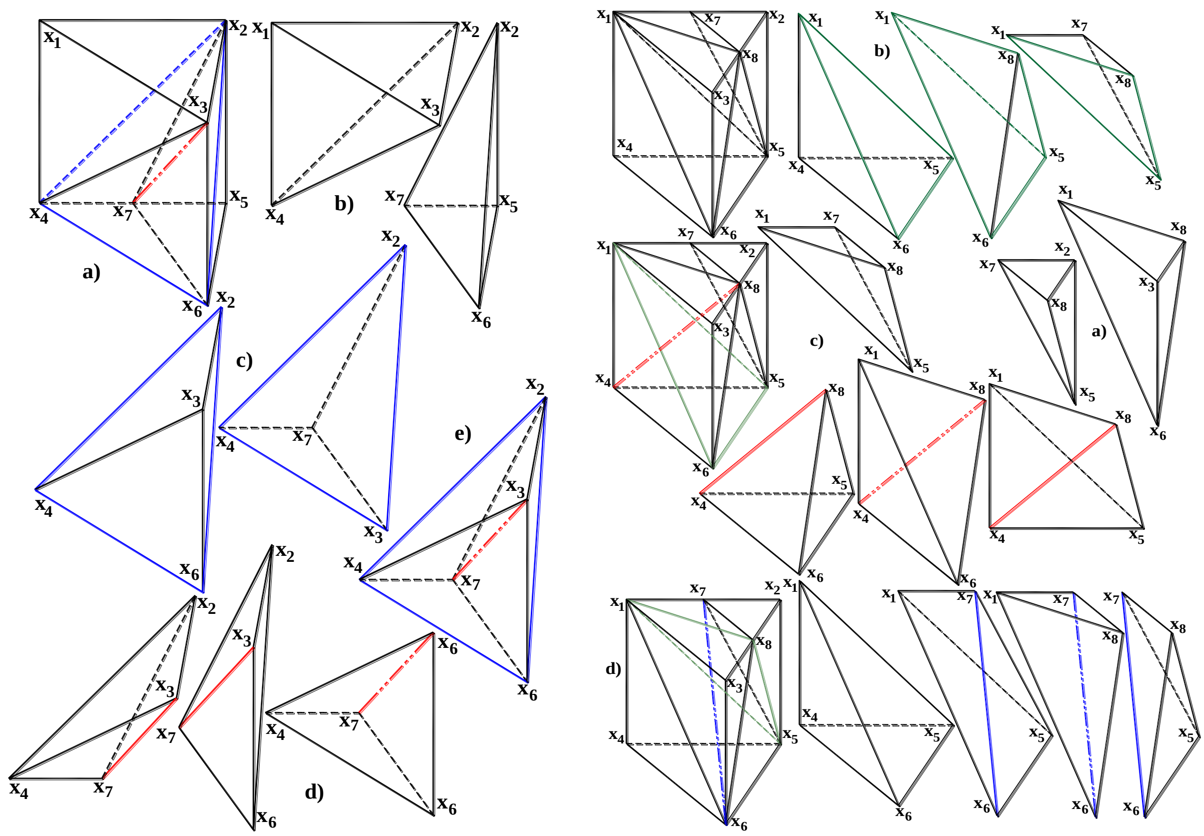

Fig. 2. To the left: 2 variants of polyhedration for a compound x_7 and competition of the diagonal x_3x_7 with the plane $x_2x_4x_6$ (a): common tetrahedrons $x_1x_2x_3x_4$, $x_2x_5x_6x_7$ (b); additional tetrahedrons $x_2x_3x_4x_6$, $x_2x_4x_6x_7$, if to divide by the plane $x_2x_4x_6$ (c); additional tetrahedrons $x_2x_3x_4x_7$, x$_2$x$_3$x$_6$x$_7$, x$_3$x$_4$x$_6$x$_7$, if to divide by the common diagonal x_3x_7 of 3 faces $x_2x_3x_7$, $x_3x_4x_7$, $x_3x_6x_7$ (d); undivided micro-complex $x_2x_3x_4x_6x_7$ (e). To the right: 3 variants of polyhedration for binary compounds x_7, x_8: 2 common tetrahedrons $x_1x_3x_6x_8$, $x_2x_5x_7x_8$ (a); 3 additional tetrahedrons $x_1x_4x_5x_6$, $x_1x_5x_6x_8$, $x_1x_5x_7x_8$, if to divide without inner diagonals (b), it is the only variant, identified by the ZK Algorithm; 4 additional tetrahedrons $x_1x_4x_5x_8$, $x_1x_4x_6x_8$, $x_4x_5x_6x_8$, $x_1x_5x_7x_8$, if to divide by the diagonal x_4x_8 and its faces $x_1x_4x_8$, $x_4x_5x_8$, $x_4x_6x_8$ (c); 4 additional tetrahedrons $x_1x_4x_5x_6$, $x_1x_5x_6x_7$, $x_1x_6x_7x_8$, $x_5x_6x_7x_8$, if to divide by the diagonal x_6x_7 and its faces $x_1x_6x_7$, $x_5x_6x_7$, $x_6x_7x_8$ (d).

The adjacency list after multiplication and inverse gives a tetrahedron $x_3x_6x_{11}x_{12}$, two inner planes $x_3x_9x_{10}+x_3x_4x_5$, a fragment of upper face $x_3x_7x_8$ and 4 symmetric pairs of triangles on the quadrangle faces $x_1x_7x_9+x_2x_8x_{10}$, $x_3x_7x_9+x_3x_8x_{10}$, $x_3x_4x_9+x_3x_5x_{10}$, $x_3x_4x_{11}+x_3x_5x_{12}$. To underline the existence of micro-complexes with solid solutions and to fulfill the dividing to the finish, it is necessary to use some virtual diagonals not only on corresponding faces (or their fragments), but on the diagonal plane $D_1D_3D_4D_2=x_7x_9x_{10}x_8$ too. Then elements $r_{1,8}$, $r_{1,10}$, $r_{2,7}$, $r_{2,9}$, $r_{4,10}$, $r_{4,12}$, $r_{5,9}$, $r_{5,11}$, $r_{7,10}$, $r_{8,9}$ become equal to 1 (they are deleted from R_L) and the multiplication $(x_1+x_3x_4x_5x_6x_{11}x_{12})\cdot$ $\cdot(x_2+x_3x_4x_5x_6x_{11}x_{12})(x_4+x_6x_7x_8)(x_5+x_6x_7x_8)(x_6+x_7x_8x_9x_{10})(x_7+x_{11}x_{12})(x_8+x_{11}x_{12})(x_9+x_{11}x_{12})(x_{10}+x_{11}x_{12})=$ $=x_1x_2x_4x_5x_7x_8x_9x_{10}+x_1x_2x_6x_7x_8x_9x_{10}+x_1x_2x_6x_7x_8x_{11}x_{12}+x_1x_2x_4x_5x_6x_{11}x_{12}+x_3x_4x_5x_6x_{11}x_{12}$ after inverse has as a result a tetrahedron $x_3x_6x_{11}x_{12}$, one 6-vertex $x_1x_2x_7x_8x_9x_{10}$ micro-complex and three 5-vertex $x_3x_4x_5x_{11}x_{12}+x_3x_4x_5x_9x_{10}+x_3x_7x_8x_9x_{10}$ micro-complexes of solid solutions.

ZK Algorithm limitations

Algorithm can not divide the polyhedron with inner points [2, 6, 7] and with competition of inner diagonals and planes. For instance, two variants of polyhedration in the quaternary reciprocal system with a binary compound x_7 in the ternary system $x_4x_5x_6$ (Fig. 2, left) are possible because of competition between the diagonal x_3x_7 and the plane $x_2x_4x_6$. Polyhedration gives two tetrahedrons in both cases and two or three additional tetrahedrons. But the ZK Algorithm fulfills the only polyhedration by the plane $x_2x_4x_6$. If to write in the adjacency matrix $r_3r_7=1$, then the ZK Algorithm gives, except 2 common tetrahedrons, a micro-complex $x_2x_3x_4x_6x_7$ only. Analogously, the ZK Algorithm in the system with two binary compounds x_7 and x_8 in the ternary system $x_1x_2x_3$ (Fig. 2, right) from 3 probable variants (without inner diagonal or with one of two diagonals, x_4x_8 or x_6x_7) identifies the only variant without diagonal.

Topological rules for A,B,C||X,Y polyhedrons

If to present a trigonal prism of the quaternary reciprocal system A,B||X,Y,Z (or A,B,C||X,Y) as a graph and to describe it by the adjacency matrix, then for V vertexes of the graph and J its joinings (connections) their numbers are equal to: $V=V_0+V_E+V_F+V_I$ and $J=J_E+J_F+J_I$, (1)
where V_0 are the original vertexes of the trigonal prism A,B||X,Y,Z, V_E - points (binary compounds) on its *E*dges, J_E - *E*dges (or their fragments – binary systems without compounds); V_F are points (ternary compounds) on *F*aces, J_F - diagonals on *F*aces, S_F - 2D *S*implexes (triangles) on *F*aces; V_I are points (quaternary compounds) *I*nside the prism, J_I - *I*nner diagonals, S_I - *I*nner diagonal planes (2D simplexes), T - 3D simplexes or *T*etrahedrons. As an original trigonal prism of a quaternary reciprocal system has $V_0=6$ vertexes, $J_E=9$ edges and five faces (two triangles and three squares), then its edges are divided by V_E points to $J_E=9+V_E$ segments (simple binary systems). Numbers of diagonals (J_F) and simplexes (S_F) on faces, inner 2D planes-simplexes (S_I) and 3D tetrahedrons-simplexes (T) are expressed [6,7] as): $J_F=3+2V_E+3V_F$, $S_F=8+2V_E+2V_F$, $S_I=2+V_E+V_F-2V_I+2J_I$, $T=3+V_E+V_F-V_I+J_I$. (2)

So, to define the quantity of tetrahedrons-simplexes T and inner planes S_I in advance, it is enough to know the numbers of binary V_E, ternary V_F, quaternary V_I compounds and inner diagonals J_I.

New algorithm of polyhedration

Because of ZK Algorithm shortcomings, the New Algorithm has been elaborated. In contrast to the ZK Algorithm the new one works with “1” elements of the adjacency matrix. It consists of three steps: 1) All connections x_ix_j, including all possible inner diagonals (lines, connecting every binary compound of both triangular faces of the prism with opposite vertexes), are written; 2) All possible planes $x_ix_jx_k$ of three types are formed: S_F planes on faces, S_I^* inner planes without inner diagonals on their sides and S_I^{**} inner planes, connected with possible inner diagonals. The last type of planes (S_I^{**}) is analyzed in accordance to formulas (2), which estimate all probable variants of polyhedration and confirm only those combinations of S_I^{**} planes, that produce together with S_F and S_I^{*} all possible tetrahedrons; 3) All S_F, S_I^{*} and selected at the second step planes S_I^{**} form tetrahedrons of two types, with and without the inner diagonals. The New Algorithm put out all possible variants of polyhedration at competition of inner diagonal elements: lines and planes. So, the last step is to confirm experimentally which of inner diagonals and planes must participate in polyhedration. It permits to find tetrahedrons, which the ZK Algorithm doesn't identify.

Problems with the polyhedration of K,Li,Ba||F,WO$_4$ system

Six polyhedron vertexes and 4 compounds [8] are enumerated: x_1=KF, x_2=LiF, x_3=BaF$_2$, x_4=K$_2$WO$_4$, x_5=Li$_2$WO$_4$, x_6=BaWO$_4$, x_7=D$_1$=LiBaF$_3$SO$_4$, x_8=D$_2$=K$_3$FWO$_4$, x_9=D$_3$=LiKWO$_4$, x_{10}=D$_4$=K$_2$Ba(WO$_4$)$_2$ (Fig. 3). As any binary compound on the side of a ternary system (excluding the common edges of two reciprocal systems) should be connected with opposite vertexes of the prism, then the compound x_7=D$_1$=LiBaF$_3$SO$_4$ may be connected with vertexes x_4, x_8, x_9, x_{10}, and x_9 – with x_3, x_7, and x_{10} - with x_2, x_7 (Fig. 3). Inner diagonals must not be intersected inside the prism, so it is necessary to enquire all possible variants of their intersections (analytically, by the resolving of corresponding equations) and then to analyze them. Results of types "inner cross-section exists" ("+") or "it is absent" ("–") are in the Table 1. (Obviously, lines x_4x_7, x_7x_8, x_7x_9, x_7x_{10} have a common point x_7, lines x_2x_{10} and x_7x_{10} – common point x_{10}, lines x_3x_9 and x_7x_9 – common point x_9, but the inner intersections on the faces or inside the prism are prohibited).

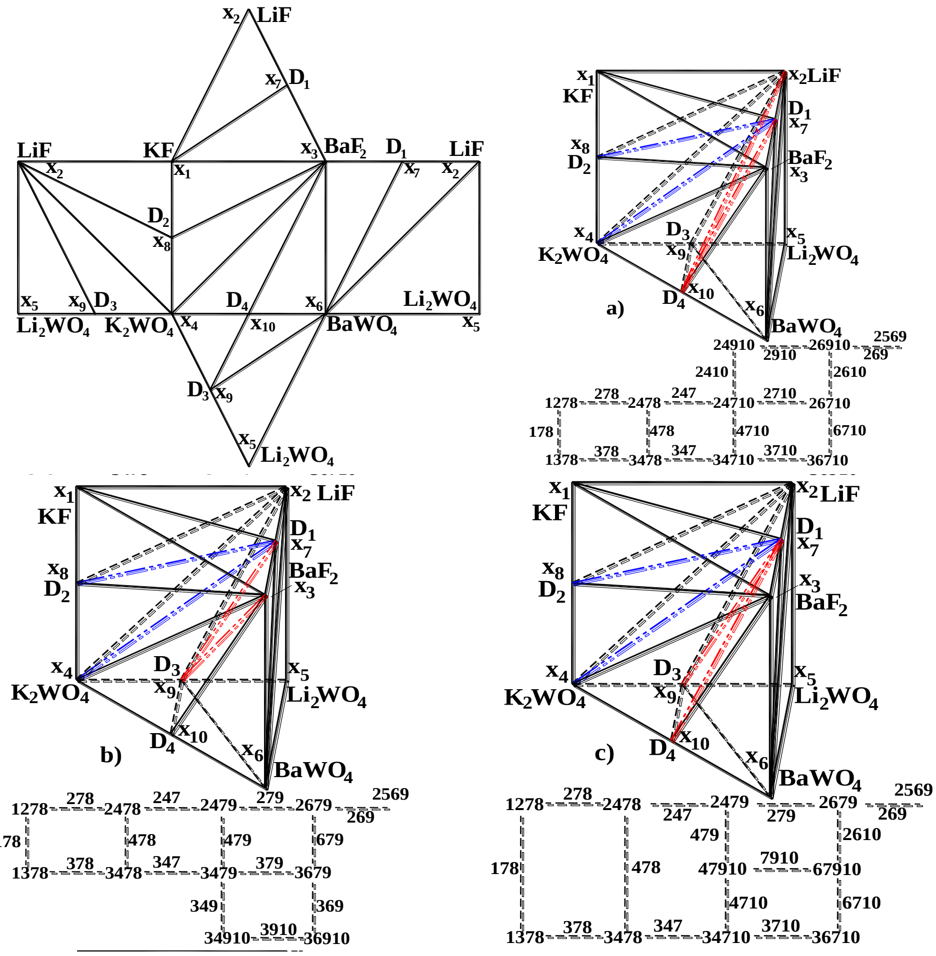

Fig. 3. Triangulated faces of prism K,Li,Ba||F,WO$_4$ and 3 variants of its tetrahedration by alternative inner diagonals: $x_2x_4x_9x_{10}$, $x_2x_4x_7x_{10}$, $x_3x_4x_7x_{10}$, $x_2x_6x_9x_{10}$, $x_2x_6x_7x_{10}$, $x_3x_6x_7x_{10}$ by x_2x_{10}+x_7x_{10} (a); $x_2x_4x_7x_9$, $x_3x_4x_7x_9$, $x_3x_4x_9x_{10}$, $x_2x_6x_7x_9$, $x_3x_6x_7x_9$, $x_3x_6x_9x_{10}$ by x_3x_9+x_7x_9 (b); $x_2x_4x_7x_9$, $x_3x_4x_7x_{10}$, $x_4x_7x_9x_{10}$, $x_2x_6x_7x_9$, $x_6x_7x_9x_{10}$, $x_3x_6x_7x_{10}$ by x_7x_9+x_7x_{10} (c).

Table 1. Variants of possible cross-sections for inner diagonals (Fig. 3)

	x_2x_{10}	x_3x_9	x_4x_7	x_7x_8	x_7x_9	x_7x_{10}
x_2x_{10}	*	+	–	–	+	–
x_3x_9		*	–	–	–	+
x_4x_7			*	–	–	–
x_7x_8				*	–	–
x_7x_9					*	–

As lines x_4x_7 and x_7x_8 have no inner intersections, they are the doubtless diagonals. The line x_2x_{10} is intersected with x_3x_9 and x_7x_9. Alternative to x_2x_{10} diagonal, a x_3x_9 one can coexist only with the diagonal x_7x_9. (They coexist with $x_4x_7+x_7x_8$). So, it is necessary to testify the variants with alternative diagonals x_2x_{10} and x_3x_9: $x_2x_{10}+x_4x_7+x_7x_8+x_7x_{10}$, $x_3x_9+x_4x_7+x_7x_8+x_7x_9$. Third variant has no both alternative diagonals x_2x_{10} and x_3x_9: $x_4x_7+x_7x_8+x_7x_9+x_7x_{10}$.

Table 2. Enquiring of possible polyhedrons variants according to formulas (2). Variants at J_I>4 are impossible because of x_2x_{10} intersection with x_3x_9, x_7x_9 and x_3x_9 - with x_7x_{10}

J_I	Diagonals	Inner planes	Tetrahedrons $S_I=2+P_E+2J_I$
0	-	$x_2x_6x_9$	***1<6***
1	x_7x_8	$x_2x_6x_9+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8$	1+3=***4<8***
1	x_7x_{10}	$x_2x_6x_9+x_3x_7x_{10}$, $x_6x_7x_{10}$	1+2=***3<8***
2	$x_7x_8+x_7x_{10}$	$x_2x_6x_9+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8+x_3x_7x_{10}$, $x_6x_7x_{10}$	1+3+2=***6<10***
2	$x_2x_{10}+x_7x_{10}$	$x_2x_6x_9+x_2x_4x_{10}$, $x_2x_6x_{10}$, $x_2x_7x_{10}$, $x_2x_9x_{10}+x_3x_7x_{10}$, $x_6x_7x_{10}$	1+4+2=***7<10***
2	$x_3x_9+x_7x_9$	$x_2x_6x_9+x_3x_4x_9$, $x_3x_6x_9$, $x_3x_7x_9$, $x_3x_9x_{10}+x_2x_7x_9$, $x_6x_7x_9$, $x_7x_9x_{10}$	1+4+3=***8<10***
3	$x_2x_{10}+x_7x_8++x_7x_{10}$	$x_2x_6x_9+x_2x_4x_{10}$, $x_2x_6x_{10}$, $x_2x_7x_{10}$, $x_2x_9x_{10}+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8+x_3x_7x_{10}$, $x_6x_7x_{10}$	1+4+3+2= ***=10<12***
3	$x_3x_9+x_7x_8+x_7x_9$	$x_2x_6x_9+x_3x_4x_9$, $x_3x_6x_9$, $x_3x_7x_9$, $x_3x_9x_{10}+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8+x_2x_7x_9$, $x_6x_7x_9$, $x_7x_9x_{10}$	1+4+3+3= ***=11<12***
4	$x_2x_{10}+x_4x_7+$ $+x_7x_8+x_7x_{10}$	$x_2x_6x_9+x_2x_4x_{10}$, $x_2x_6x_{10}$, $x_2x_7x_{10}$, $x_2x_9x_{10}+x_2x_4x_7$, $x_3x_4x_7$, $x_4x_7x_8$, $\boldsymbol{x_4x_7x_9}$, $x_4x_7x_{10}+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8+x_3x_7x_{10}$, $x_6x_7x_{10}$	1+4+5+3+2= **=15–1=14=14** ***$x_4x_7x_9$ is excluded***
4	$x_3x_9+x_4x_7+$ $+x_7x_8+x_7x_9$	$x_2x_6x_9+x_3x_4x_9$, $x_3x_6x_9$, $x_3x_7x_9$, $x_3x_9x_{10}+x_2x_4x_7$, $x_3x_4x_7$, $x_4x_7x_8$, $x_4x_7x_9$, $\boldsymbol{x_4x_7x_{10}}+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8+x_2x_7x_9$, $x_6x_7x_9$, $\boldsymbol{x_7x_9x_{10}}$	1+4+5+3+3= **=16–2=14=14** ***$x_4x_7x_{10}$, $x_7x_9x_{10}$ are excluded***
4	$x_4x_7+x_7x_8+$ $+x_7x_9+x_7x_{10}$	$x_2x_6x_9+x_2x_4x_7$, $x_3x_4x_7$, $x_4x_7x_8$, $x_4x_7x_9$, $x_4x_7x_{10}+x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8+x_2x_7x_9$, $x_6x_7x_9$, $x_7x_9x_{10}+x_3x_7x_{10}$, $x_6x_7x_{10}$	1+5+3+3+2=**14=14**

As the system has P_E=4 binary compounds (x_7, x_9, x_{10} are on the upper triangular face of the prism, x_8 is on its vertical edge), then, according to formulas (2): $J_E=9+P_E=13$, $J_F=3+2P_E=11$, $S_F=8+2P_E=16$, numbers of inner diagonals J_I (x_2x_{10}, x_3x_9, x_7x_4, x_7x_8, x_7x_9 and x_7x_{10}) may vary from 0 to 6, inner planes $S_I=2+P_E+2J_I$ from 6 at J_I=0 to 18 at J_I=6, 3D simplexes $T=3+P_E+J_I$ from 7 at J_I=0 to 13 at J_I=6.

Step 1: All $J_E+J_F+J_I$=13+11+6=30 connections are written:

- J_I=6 possible inner diagonals x_2x_{10}, x_3x_9, x_4x_7, x_7x_8, x_7x_9, x_7x_{10};
- J_E=13 edges x_1x_2, x_1x_3, x_1x_8, x_2x_5, x_2x_7, x_3x_6, x_3x_7, x_4x_8, x_4x_9, x_4x_{10}, x_5x_6, x_5x_9, x_6x_{10};
- J_F=11 diagonals on faces x_1x_7, x_2x_4, x_2x_6, x_2x_8, x_2x_9, x_3x_4, x_3x_8, x_3x_{10}, x_6x_7, x_6x_9, x_9x_{10}.

Step 2: All permitted planes (37 2D simplexes) are formed from 30 connections:

- S_F=16 planes on faces ($x_1x_2x_7$, $x_1x_3x_7$), ($x_4x_9x_{10}$, $x_5x_6x_9$, $x_6x_9x_{10}$), ($x_1x_3x_8$, $x_3x_4x_8$, $x_3x_4x_{10}$, $x_3x_6x_{10}$), ($x_1x_2x_8$, $x_2x_4x_8$, $x_2x_4x_9$ $x_2x_5x_9$), ($x_2x_5x_6$, $x_2x_6x_7$, $x_3x_6x_7$);
- S_I^*=1 plane $x_2x_6x_9$ inside the prism without inner diagonals;
- S_I^{**}=20 planes with six different inner diagonals: x_2x_{10} ($x_2x_4x_{10}$, $x_2x_6x_{10}$, $x_2x_7x_{10}$, $x_2x_9x_{10}$), x_3x_9 ($x_3x_4x_9$, $x_3x_6x_9$, $x_3x_7x_9$, $x_3x_9x_{10}$), x_4x_7 ($x_2x_4x_7$, $x_3x_4x_7$, $x_4x_7x_8$, $x_4x_7x_9$, $x_4x_7x_{10}$), x_7x_8 ($x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8$), x_7x_9 ($x_2x_7x_9$, $x_6x_7x_9$, $x_7x_9x_{10}$), x_7x_{10} ($x_3x_7x_{10}$, $x_6x_7x_{10}$).

***Step 3*:** variants of polyhedration with 4 inner diagonals can be realized.
The inner plane $x_2x_6x_9$ and S_F=16 planes on faces together with S_I=2+P_E+2J_I=14 inner planes at J_I=4 diagonals produce T=3+P_E+J_I=11 (P_E=J_I=4) tetrahedrons (Fig. 6): - a tetrahedron $x_2x_5x_6x_9$ - without inner diagonals;
- 4 tetrahedrons $x_1x_2x_7x_8$, $x_1x_3x_7x_8$, $x_2x_4x_7x_8$, $x_3x_4x_7x_8$, produced by diagonals x_4x_7+x_7x_8;
- 6 tetrahedrons (on dependence of a choice of second pair of diagonals).

Conclusions

1) Software, based by the ZK Algorithm [4, 5], had been elaborated. It consists of four steps: - to represent n-component system as a graph, - to record the adjacency list with the adjacency matrix zero elements, - to multiply the adjacency list elements accounting the absorption law, - to fulfill inversion; - to sort out all possible polyhedration variants and to drop the ones, non-real geometrically or non-supported by experiment. Systems with solid solutions requires additional virtual diagonals. Polyhedration with inner isolated points is fulfilled in two stages: without inner points at first and with inner points in micro-complexes.

2) Interrelations between the number of inner diagonal planes and simplexes on the one hand and non-zero elements of the adjacency matrix on the other hand had been got. They are very useful for the original data and program output verification and give a possibility to estimate the polyhedration result a priory.

3) The New Algorithm has been elaborated. It may be applied for polyhedration of quaternary and more complex multicomponent systems (including the reciprocal ones) and it is able to identify all variants of polyhedration, including situations, when the ZK Algorithm can not “recognize” some simplexes.

4) Topological Rules embrace interrelations between all geometrical elements of polyhedron, including its binary, ternary subsystems and binary, ternary, quaternary compounds (systems with quaternary compounds were not yet analyzed).

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