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GRAPHICAL PRESENTATION METHOD OF CRYSTALLOCHEMICAL FORMULAS OF TWO- AND THREE-BEDDED MINERALS

(*Fig. 1—8*)

Abstract: In the paper a method of graphical presentation of two- and three-bedded hydrosilicates is described. On the basis of this method interrelations between minerals of mentioned two groups are investigated.

Introduction

Among important characterizations of clay minerals their crystallochemical formulas belong obtained by conversion of complete chemical analysis. The crystallochemical formulas of minerals of group of two-bedded silicates (phyllosilicates) with two-bedded structure essentially represent four changing chemical constituents with regard to possible isomorphism. Crystallochemical formulas of bedded silicates with more than four constituents, at which substitution of chemical constituents is still possible, become with graphical presentation not only clear but also offer opportunity of quick comparison.

The subject of the paper is graphical presentation of two- and three-bedded silicates from their crystallochemical formulas.

Graphical Presentation of Two-Bedded Silicates

1. Crystallochemical Formulas of Halloysite and Kaolinite

The substantial structure units of kaolinite lattice is according to S. B. Hendricks (1938) one tetrahedral bed — Si_4O_{10} in connection with common four oxygens with one octohedral bed $Al_4(OH)_8$, the ideal crystallochemical formula corresponds to $Al_4\,[Si_4O_{10}]\,[OH]_8$.

Halloysite is of identical crystal structure as kaolinite. There is the difference only that halloysite containts four water molecules bound between the substantial structural two beds, with water content changeable from four molecules to dehydrate. Besides that isomorphism of silicon in tetrahedral and of aluminium in octahedral bed is possible. Therefore its general formula may be written as follows:

$Al_{m-n}\,(Al_nSi_{4n})\,O_{10}\,(OH)_8\,.\,4H_2O$

and as ideal formula

$Al_4\,[Si_4O_{10}]\,[OH]_8\,.\,4H_2O$

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2. Calculation of Crystallochemical Formulas

The calculation of crystallochemical formulas we carry out in the following way:

Mass percentage of chemical constituents ascertained by chemical analysis (tab. 1, column 1) are converted into percentage of atoms (column 2). From mass percentage of atoms atomic quotients (column 3) are calculated as the ratio of mass percentage to atomic weights and converted into ion numbers (column 4). Ion numbers are converted in relation to $(O + OH) = 18$ (column 5). In this way we obtein the numerical stechiometrical ratio of the main chemical constituents of halloysite and kaolinite for the crystallochemical formula. As an example we mention the calculation of crystallochemical formula of halloysite of ideal chemical composition (tab. 1).

The crystallochemical formula of halloysite:

$Al_4 [Si_4O_{10}] [OH]_8 . 4H_2O$

For graphical presentation of crystallochemical formulas we chose 7 halloysite samples from classical localities of eastern Slovakia and one sample each for comparison of halloysite (1) and kaolinite (7) of ideal chemical composition (tab. 2).

We started from changeable values of four main crystallochemical constituents: So, Al, (OH), H_2O (interstratal). The fifth value of crystallochemical constituent O being of value 0_{10} in the crystallochemical formula, is a constant crystallochemical constituent and therefore we did not take it into consideration in graphic presentation.

For clearness we converted the given values of crystallochemical formula to sum value 100 and these we employed then in further graphic solution.

3. Illustration of Mixture with Four Constituents in Vectorial Projection

For illustration of systems of four kinds tetrahedron is used. The illustration of regular tetrahedron is particularly advantageous in vectorial projection (J. Klimčík 1966). For this purpose we choose the equilateral triangle ABC as base in projection plane π and determine its centre D (fig. 1). We put the

Table 1

chemical constituents	1 mass %	crystallochemical constituents	2 mass %	3 atomic quotients	4 ion numbers	amount of ion numbers for $(O+OH = 18)$		
SiO_2	40,84	Si	19,08	0,6799	679,9		4	
Al_2O_3	34,66	Al	18,34	0,6800	680,0		4	
H_2O^+	12,25	OH	23,14	1,3610	1361,0	3060,0	8	18
H_2O^-	12,25	O	27,19	1,6990	1699,0		10	
		H_2O^-	12,25	*0,6855	685,5		4	

* molecular quotient

Table 2

Sample No.	designation of sample	Si	Al	OH	H_2O	concersion to 100					crystallochemical formula
						Si b	Al c	OH d	H_2O a	together	
1	Ideal halloysite	4,00	4,00	8,00	4,00	20,0	20,0	40,0	20,0	100	$Al_4[Si_4O_{10}]\ [OH]_8\ .\ 4H_2O$
2	Halloysite Djebal, Debar (Algeria)	3,94	4,04	8,00	4,00	19,7	20,2	40,1	20,0	100	$Al_{4.04}[Si_{3.94}O_{10}]$ $[OH]_8\ .\ 4H_2O$
3	Halloysite Eureka, Utah	3,84	4,04	8,00	4,00	19,3	20,3	40,3	20,1	100	$Al_{4.04}[Si_{3.84}O_{10}]$ $[OH]_8\ .\ 4H_2O$
4	Halloysite Eastern Slovakia	3,89	3,81	7,97	4,31	19,5	19,0	39,9	21,6	100	$Al_{3.81}[Si_{3.89}O_{10}]$ $[OH]_{7.97}\ .\ 4{,}31\ H_2O$
5	Halloysite Eastern Slovakia	3,79	3,64	7,98	4,66	18,9	18,1	39,8	23,2	100	$Al_{3.64}[Si_{3.79}O_{10}]$ $[OH]_{7.98}\ .\ 4{,}66\ H_2O$
6	Halloysite Eastern Slovakia	3,82	4.08	7,53	3,26	20,4	21,8	40,3	17,5	100	$Al_{4.08}[Si_{3.82}O_{10}]$ $[OH]_{7.53}\ .\ 3{,}26\ H_2O$
7	Ideal kaolinite	4,00	4,00	8,00	—	25,0	25,0	50,0	—	100	$Al_4[Si_4O_{10}]\ [OH]_8$
8	Halloysite Vyshkovo (USSR)	3,83	3,58	8,00	3,00	20,8	19,5	43,4	16,3	100	$Al_{3.58}[Si_{3.83}O_{10}]$ $[OH]_8\ .\ 3H_2O$
9	Halloysite Berehovo (USSR)	4,41	3,39	8,00	1,45	25,7	19,6	46,4	18,3	100	$Al_{3.39}[Si_{4.41}O_{10}]$ $[OH]_8\ .\ 1{,}45H_2O$

plane perpendicular to projection π (thus also to the base) through one of the heights of the base, e. g. BU and let it down to projection plane π in the way that we erect a perpendicular to BU in point D and intersect it by an arch with centre in B and of radius $r = \overline{BC}$. The real distance of the tetrahedron height is $\overline{D(D)}$. The vectorial projection may form with the height of tetrahedron base CZ an angle of 45° and in this way we obtained clear constructions. In the direction of projecting we carry over the real height of tetrahedron from point D so that $\overline{D(D)} = \overline{DD'}$ (in dimensioned projection we should ascribe to point D dimension equal to $\overline{D(D)}$ and here we drew the vector $\overline{DD'}$, D is the initial point of vector and D′ the terminal point presented by the vector). The points A, B, C are in projection plane π, therefore their vector is zero and consequently $A \equiv A'$, $B \equiv B'$, $C \equiv C'$. In the next for the purpose of simplicity we are going to designate them A, B, C only.

The tetrahedron in fig. 1 represents a spatial model. Its peaks A, B, C, D represent constituents. The edges of the tetrahedron AB, AC, AD, BC, BD, CD

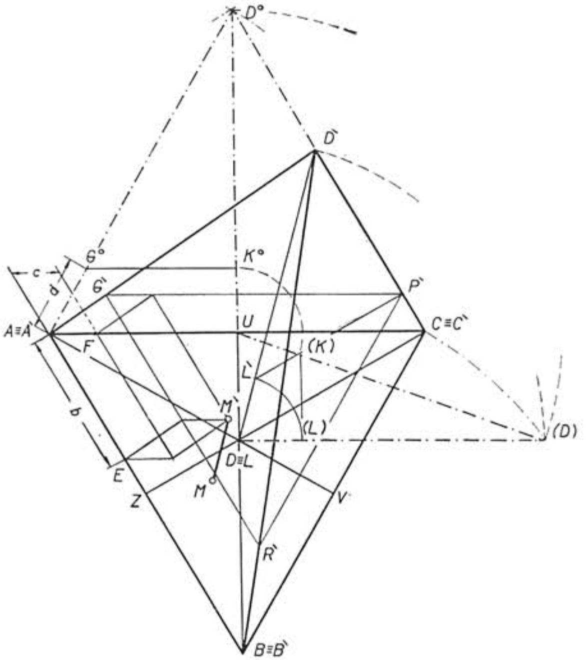

Fig. 1. Presentation of system with four constituents.

are axes of concentrations of corresponding systems of two kinds and the points U, V, Z represent concentrations of binary mixtures of the determined system. The faces ABD, BCD, ACD, ABC are triangles of constituents concentrations. An arbitrary point at the face of the mixture tetrahedron consists of tree constituents (e. g. kaolin 7 in fig. 3).

All points inside the tetrahedron (point M for instance) will correspond to mixtures with four constituents of controlling concentrations. In fig. 1 presentation of mixture with four constituents is realized.

Let us have a mixture containing a = 28,5 % of constituent A, b = 39 % of constituent B, c = 12,5 % of constituent C, d = 20 % of constituent D, $a+b+c+d = 100\ \%$.

We divide the edges of tetrahedron into 100 equal parts; in our case the edge is 100 mm long. For solution of further tasks it is adventageous to construct several tetrahedrons in advance, the lest on tracing-paper and to carry out constructions in them.

If we draw from peak A the abscissa c on AC to point F, b on side AB to E, d on side AD to point G and draw planes parallel to faces ACD, ABD, ABC through the points F, E, G they intersect in the point M inside the tetrahedron. This point M presents the mixture of given composition. Let us choose the point A as the origin of vectorial coordinal system and the edges AB, AC, AD as coordinal axes, the constituents B, C, D, expressed by percentage (b, c, d) will be the coordinates of point M.

The edges AB, AC, which are sides of the tetrahedron base, situated in the projection plane, are presented in real size of the chosen scale. Therefore we present the per cent content of constituents B ($b = \overline{AE}$), C ($c = \overline{AF}$) in real size. As a consequence of misrepresented edges AD, BD, CD we must shorten the component $d = \overline{AG}$.

For this purpose we turn the face ACD into projection plane π and obtain the equilateral triangle AC°D. From point A we draw the abscissa $d = \overline{A^\circ G}$ on side $\overline{A^\circ D}$ and turn the triangle AC°D into previous position. In order to be able to construct terminal projection G′ of point G on terminal projection AD′ of edge AD we draw a parallel with AC through point G°, which intersects height U°D of the turned face in point °K. We carry abscissa U°K from point U over U (D) to point (K) and the perpendicular to D (D) erected from the intersects the abscissa in point (L). We carry abscissa D (L) over the height DD′ of tetrahedron to point L′. We put the PRG parallel to π through terminal point L′ of the point L in a way that first we draw through point L the straight L′P parallel to ZG, which intersects terminal projection C′D′ of edge CD of the tetrahedron in point P′. The straight line P′G′∥AC intersects terminal projection A′D′ of edge AD in seeked terminal projection G′ of point G. The abscissa $\overline{L(L)} = \overline{LL'}$ detedmines the distance of point M from tetrahedron base.

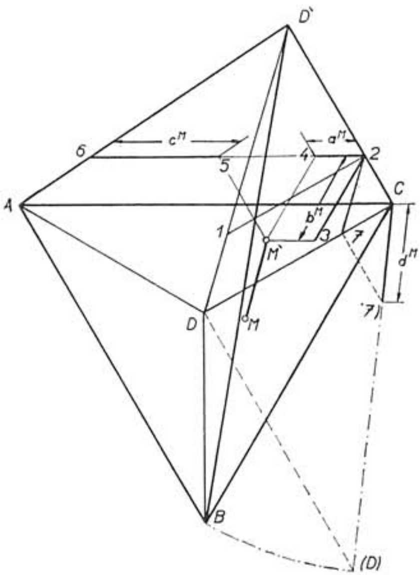

Fig. 2. Determination of per cent composition of given system.

The parallelepipedon of coordinates constructed over the abscissas AF, AE, AG′ determines the peak (i. e. M′M = LL′) that illustrates the point corresponding to mixture seeked for.

4. Percentage Determination of Constituents of Given Mixture

Percentage representation of mixture constituents corresponding to point M inside the tetrahedron can be found by aid of perpendiculars to its faces drawn through the point mentioned (J. Klimčík 1966). We present graphically a very simple determination of coordinates of point M (fig. 2).

We put a plane parallel to π (the plane is not indicated) through point M. The secant of this plane with face CDD′ is the straight line 1 2. parallel to initial projection DC, at which $\overline{MM'} = \overline{D1}$.

If we draw through point 2 a straight line parallel to edge CB and through point M′ a straigh line parallel to edge AC, they intersect in point 3, where $\overline{2\,3} = b^M$ and $\overline{M'3}$ or $\overline{4\,2} = a^M$. After plotting of point 7 (2 7 ∥ DD′; 7 lies on CD) and determination (7) with letting down is on $C(D)d^M = \overline{C(7)}$. The coordinate (constituent) $c^M = \overline{6\,5}$ and M′5 ∥ AB or $c^M = \overline{AB} - (a^M + b^M + d^M)$.

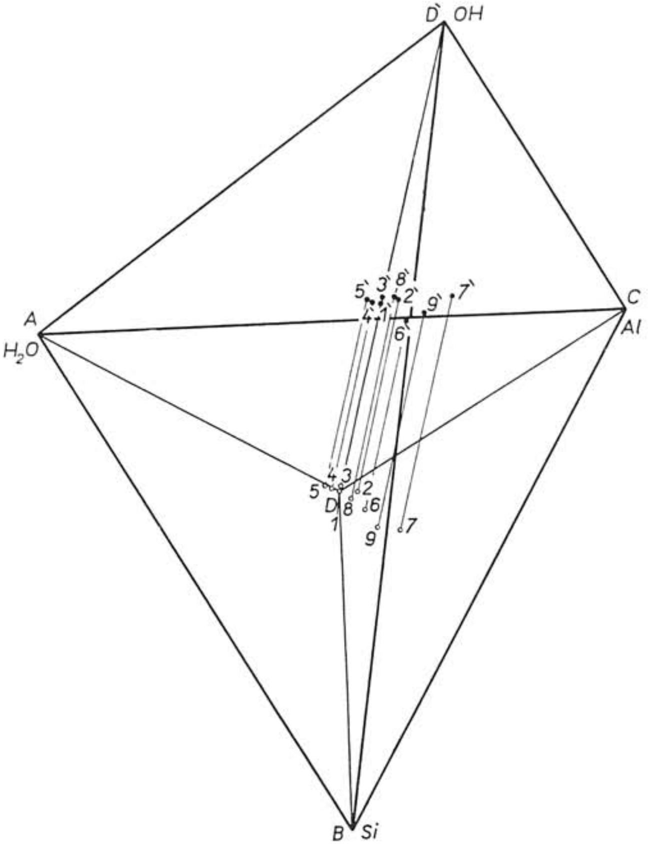

Fig. 3. Comparison of qualities of given systems of halloysite and kaolinite.

Table 3

Montmorillonite, Upton, Wyoming

chemical constituents	weight %	factor	molar fractures	
SiO_2	55,44	60,06	0,1194 = X	
Al_2O_3	20,14	51,00	0,9231 = Z	
Fe_2O_3	4,00	79,92	0,3952 = A	
MgO	2,49	40,32	0,0502 = B	
CaO	0,50	56,00	0,0618 = D	0,0888
K_2O	0,60	94,20	0,0089 . 2	
Na_2O	2,75	62,00	0,0128	

Crystallochemical formule:
$[Si_{7.77}\,Al_{0.23}]\ [Al_{3.09}\,Fe_{0.42}\,Mg_{0.51}]\ O_{10}\ [OH]_4\ [X_{1.00}]$

For the purpose of comparison of qualities of certain halloysites (see tab. 2) they were presented in above mentioned way on the basis of their crystallochemical formulas. With known choice of tetrahedron and according to crystallochemical formulas of halloysites the constituents are represented as follows: $A = H_2O = a\ {}^0/_0$, $B = Si = b\ {}^0/_0$, $C = Al = c\ {}^0/_0$, $D = OH = d\ {}^0/_0$ (fig. 3).

The individual samples are marked with numbers 1 to 9 and constructed in the known way but with twofold magnification of tetrahedron.

Graphic Presentation of Three-Bedded Silicates

1. Crystallochemical Formulas of Three-Bedded Silicates

We employed for graphic presentation crystallochemical formulas of three-bedded silicates of montmorillonoids group of dioctahedral type: montmorillonite, nontronite, beidellite; trisoctahedral type: saponite; of the group of clay micas of dioctahedral type: pyrophyllite, hydromuscovite and illite.

The crystallochemical formulas of three-bedded silicates employed can be expressed theoretically as follows:
dioctahedral type:
pyrophyllite — $[Si_8]^{IV}\ [Al_4]^{VI}\ O_{20}\ [OH]_4$
montmorillonite — $[Si_{8-x}Al_x]^{IV}\ [Al, Fe^{3+}, Mg]_4^{VI}\ [Ca, K, Na]^{XII}\ O_{20}\ [OH]_4$
montronite — $[Si_{8-x}Al_x]^{IV}\ [Al, Fe, Mg]_4^{VI}\ [Ca]^{XII}\ O_{20}\ [OH]_4$
beidellite — $[Si_{8-x}Al_x]^{IV}\ [Al, Fe^{3+}, Mg]_4^{VI}\ [Ca, K, Na]^{XII}\ O_{20}\ [OH]_4$
trioctahedral type:
talc — $[Si_8]^{IV}\ [Mg_6]^{VI}\ O_{20}\ [OH]_4$
saponite — $[Si_{8-x}Al_x]^{IV}\ [Al, Fe^{3+}, Mg]_6^{VI}\ [Ca, Na, K]^{XII}\ O_{20}\ [OH]_4$
group of dioctahedral micas:
muscovite — $[Si_6Al_2]^{IV}\ [Al_4]^{VI}\ [K_2]^{XII}\ O_{20}\ [OH]_4$
hydromuscovite — $[Si_{8-x}Al_x]^{IV}\ [Al, Fe^{3+}, Mg]_4^{VI}\ [K, Na, Ca]_2O_{20}\ [OH]_4$.
(illite)

The most methods of calculation of crystallochemical formulas from camplete chemical analysis according to the authors (W. P. Kelley 1954, C. S. Ross, S. B. Hendricks 1954) start from the fact that the substantial elementary cell of threebedded silicates has constant number of oxygens and hydroxyle groups (O_{20}; $[OH]_4$). Therefore the results obtained according to individual authors differ very little only. All methods virtually start from these assumptions about cations distribution in elementary cell:

a) cations in tetrahedral coordination [IV] are mainly Si^{4+} and Al^{3+};

b) cations in octohedral coordination [VI] are most frequently Al^{3+}, Fe^{3+}, Mg^{2+} nad Fe^{2+};

c) cations in interstratal space are mostly Ca^{2+}, Na^+, K^+, H^+;

d) the number of negative charge is equal 44.

As an example of calculation of crystallo-chemical formula according to the method of C. S. Ross, S. B. Hendricks (1945) and W. P. Kelley (1954) we mention the conversion of chemical analysis of the well-known montmorillonite from Upton, Wyoming.

In the conversion according to C. S. Ross, S. B. Hendricks (1945) it is started from the universal formula (tab. 3):

$[\mathrm{Si}_{8-x}\mathrm{Al}_{x}]^{\mathrm{IV}}[\mathrm{Al}_{a-x}\mathrm{Fe}_{b}^{3+}\mathrm{Mg}_{d}]^{\mathrm{VI}}\,\mathrm{O}_{20}\,[\mathrm{OH, F}]_{4}\,[\mathrm{X}_{0.66}]$

where $a - x + b + d \sum$ (cations with octahedral coordination)

$\mathrm{Al}_{x}^{3+} + \mathrm{Si}_{8-x}^{4+} = 8$.

Mass per cent of chemical constituents is converted to molar fractures, which are designated in calculation: Z — SiO_2 content; A — Al in tetrahedral and octohedral positions; Y — Al in tetrahedral position; B — Fe^{3+}; D — Mg.

The mean content of exchange cations is equal 0,66 — $[\mathrm{X}_{0.66}]$.

By calculation of coefficient $K = \dfrac{44-0{,}66}{3A + 3B + 2D + 4Z}$ we determine equivalent amounts of cations in elementary cell, and that:

$y = K.\ Y;\ a - x = A - Y.\ K;\ b = B.\ K;\ d = D.\ K;\ x = X.\ K.$

The substitution of cations is possible in tetrahedral bed of Si^{4+} and Al^{3+}, e. g. in muscovite, hydromuscovite, illite, beidellite as well as in octohedral bed of Al^{3+} with Fe^{3+}, Mg^{2+}, mainly in montmorillonite, nontronite, saponite, beidellite, less in hydromuscovite and illite.

In the conversion according to the method of W. P. Kelley (1954) (tab. 4) mass per cent of chemical constituents (column II) is converted to molar fractures (column III) and multiplied by the number of cations (column IV). The values obtained are multiplied by the quantivalence of cations (column V). The sum of values (column V) is converted to the value 44 (column VI) and divided by the quantivalence of corresponding cation (column VII), whereby values for the calculation of crystallochemical formula are obtained (column VIII).

Free negative charges originated by substitution are compensated by cations in interstratal space.

Table 4

I	II	III	IV	V	VI	VII	VIII
SiO_2	55,41	0,9231	0,9231	3,6924	30,8190	7,704	7,71
Al_2O_3	20,14	0,1976	0,3952	1,1856	9,8957	3,2986	3,30
Fe_2O_3	4,00	0,0251	0,0502	0,1506	1,2570	0,419	0,42
MgO	2,49	0,0618	0,0618	0,1236	1,1236	0,5158	0,52
CaO	0,50	0,0089	0,0089	0,0178	0,1786	0,0743	0,08
K_2O	0,60	0,0064	0,0128	0,0128	0,1068	0,1068	0,11
Na_2O	2,75	0,0444	0,0888	0,0888	0,7418	0,7418	0,74
	—	—	—	5,2716	44,000	—	—

Crystallochemical formula:

$[\mathrm{Si}_{7.71}\mathrm{Al}_{0.29}]\ [\mathrm{Al}_{3.01}\,\mathrm{Fe}_{0.42}\,\mathrm{Mg}_{0.52}]\ [\mathrm{Ca}_{0.08}\,\mathrm{K}_{0.11}\,\mathrm{Na}_{0.74}]\ \mathrm{O}_{20}\ [\mathrm{OH}]_{4}$

The individual groups of three-bedded silicates and minerals of certain group differ in the character of ions mainly in the octahedral bed and in changeable cation substitution in tetrahedral and octohedral bed.

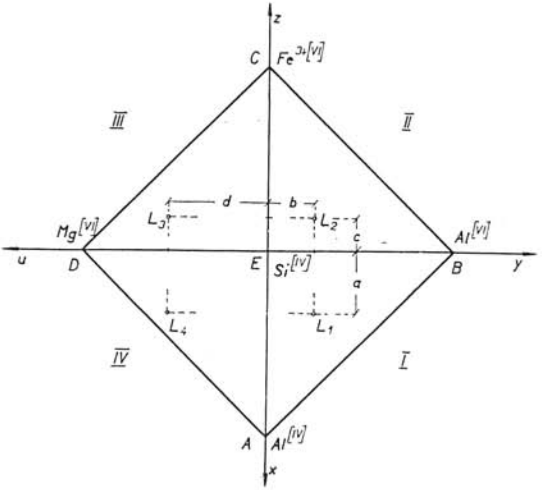

Fig. 4. Presentation of the point representing silicate in R_4.

In graphic presentation of crystallochemical formulas values mostly changeable in we therefore started from crystallochemical formulas and immediately sharing in the composition of tetrahedral and octohedral bed of elementary silicate cell. They are ions of Si^{4+} and Al^{3+} in tetrahedral bed and mainly ions of Al^{3+}, Fe^{3+}, Mg^{2+} in octohedral bed, 5 values together. Interstratal ions (Ca^{2+}, K^+, Na^+, H^+) we have not taken into consideration in graphic presentation for the reasons mentioned above. Constant number of ions O_{20} $[OH]_4$ in crystallochemical formulas also has not been taken into consideration.

Values of ions with tetrahedral and octohedral coordination as mentioned in table (V—VIII) we obtained from literature (W. A. Deer 1962, M. Gregor, B. Číčel, K. Izáková, I. Novák 1966, K. Jasmund 1955) and by proper conversion of chemical analyses.

In table (V—VIII) individual minerals are arranged in the order from minimum to maximum substitution of ions in tetrahedral and octohedral bed characteristic of one or another group of three-bedded silicates.

2. Presentation of Three-Bedded Silicate in Four-Dimension al Space R_4

In three-bedded silicate we shall, as mentioned before, consider five constituents — five points A, B, C, D, E, whihc determine the rectangular pentahedron S_5 of four-dimensional Euclid linear space R_4, delimited $\binom{5}{2} = 10$ edges, $\binom{5}{2} = 10$ faces and $\binom{5}{4} = 5$ superplanes (W. Lietzmann 1952).

We illustrate the set of five components of silicate by aid of four coordinal axes intersecting in point E and forming each an angle of 90° (fig. 4). After carrying the abscissa of the length of 100 units from point E on the axes x, y, z, u we obtain the points A, B, C, D, which represent pure components $Al^{[IV]}$, $Al^{[VI]}$, $Fe^{3+[VI]}$, $Mg^{[VI]}$. The initial point E represents component $Si^{[IV]}$. We determine an arbitrary silicate by aid of points inside the pentahedron, therefore the coordinates will be positive.

In the nex we are going to designate a point — null-dimensional space — R_0 (simplex S_1), a straight line — one-dimensional space — R_1 (S_2), a plane — two-dimensional space — R_2 (S_3), a superplane — three-dimensional space — R_3 (S_4) as subspaces of Euclid linear four-dimensional space R_4 (S_5) (Hk. de Vries 1926).

In fig. 4 point L with employing of coordinates a, b, c, d as pure constituents of A, B, C, D on axes x, y, z, u is presented, so that L_1 lies in quadrant I (xy), L_2 in quadrant II (yz), L_3 in quadrant III (zu) and L_4 in quadrant IV (ux). The joints of point projections always form a rectangle.

In four-constituents system an equilateral tetrahedron was chosen as model. In the case given a rectangular pentahedron was chosen. Each point of the pentahedron is completely determined by coordinates a, b, c, d on axes EA (x), EB (y), EG (z), ED (u) and the fifth coordinate e we find from the relation $e = 100 - (a+b+c+d)$ (P. H. Schoute 1902, H. E. Boeke 1916). Two projections of the point are dependent on the two remaining projections.

If one of the constituents is not represented, the point lies then in one of the spaces of superplane R_3, which delimit the pentahedron and two projections are on the axes. Also in four-dimensional space R_4 the relations of the centre of gravity are valid (H. E. Boeke 1916).

3. Graphic Presentation of Silicate in R_4

Individual silicates in R_4 were presented in the way mentioned above in fig. 5 according to table 5, 6, 7, 8.

In quadrant I the characteristic relation of minerals of montmorillonite group is expressed, mainly showing ions substitution in octahedral coordination and that $Al^{[VI]}$ and of minerals of hydromuscovite and illite group with substitution $Al^{[VI]}$ in octahedral coordination. In quadrant II nontronite group appears with prevailing Fe^{3+} ions in octahedral coordination. Nontronites similarly are indicated in quadrant III as well as talc and saponites. Quadrant IV is characteristic by the group of talc and saponite with Mg^{2+} ions in octohedral coordination. In this quadrant also presented groups of montmorillonite and hydromuscovite-illite appears, mainly with substitution of Si^{4+} instead of Al^{3+} in tetrahedral coordination.

In all the quadrants all groups of minerals are represented because each presented mineral of the groups mentioned even contains small amount of constituents considered so that their interrelations can be investigated in all the quadrants. Interrupted lines delimit above all minerals of certain group characterized by the position of ions in tetrahedral and octohedral coordination of crystal structure of by substitution of ions in tetrahedral and octohedral coordination.

Four points, which do not lie in the plane R_2 of four-dimensional space R_4

Fig. 5. Presentation of silicates and plotting of some silicate groups in R_4.

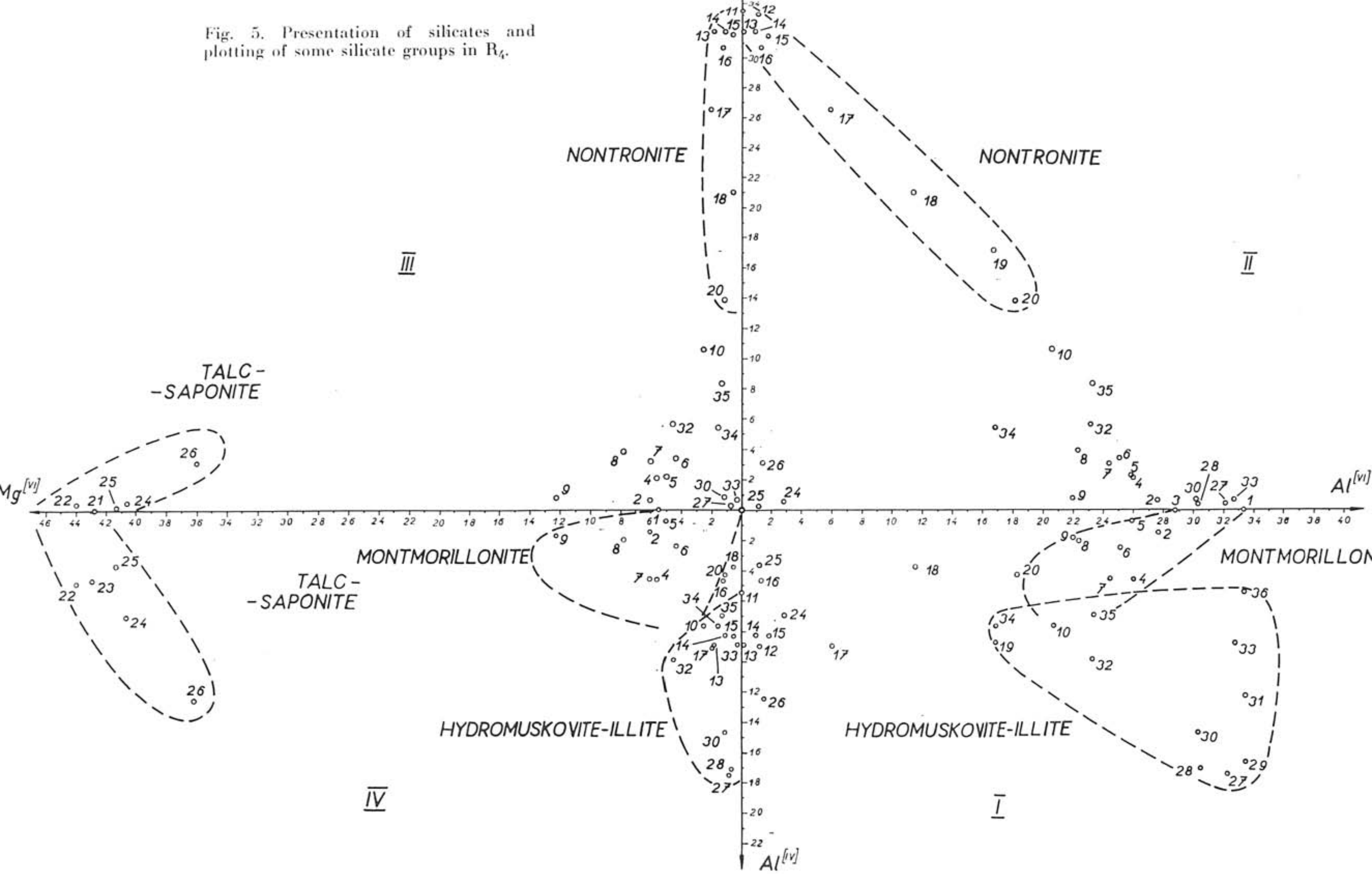

Table 5

No.	Mineral locality	Tetrahedral coordination of ions		Octahedral coordination of ions			Σ
		Si^{4+}	Al^{3+}	Al^{3+}	Fe^{3+}	Mg^{2+}	
1	pyrophyllite (theor. const.)	8,00 66,70	— —	4,00 33,30	— —	— —	12,00 100,00
2	montmorillonite Montmorillon France	7,81 64,20	0,19 1,50	3,37 27,60	0,09 0,70	0,73 6,00	12,19 100,00
3	montmorillonite (theor. const.)	8,00 61,70	— —	3,34 28,80	— —	0,66 5,50	12,00 100,00
4	montmorillonite N. Kamenica Eastern Slovakia	7,44 61,60	0,56 4,60	3,12 26,00	0,25 2,10	0,69 5,70	12,06 100,00
5	montmorillonite Kuzmice Eastern Slovakia	7,91 66,10	0,09 0,70	3,09 25,90	0,27 2,30	0,60 5,00	11,96 100,00
6	montmorillonite Upton Wyoming	7,71 64,50	0,29 2,40	3,01 25,20	0,42 3,50	0,52 4,40	11,96 100,00
7	montmorillonite Fintice Eastern Slovakia	7,45 61,80	0,55 4,60	2,95 24,40	0,39 3,20	0,72 6,00	12,06 100,00
8	montmorillonite Polkville Mississippi	7,76 64,00	0,24 2,00	2,70 22,30	0,48 3,90	0,95 7,80	12,13 100,00
9	montmorillonite Otey, California	7,78 63,20	0,22 1,80	2,69 21,90	0,10 0,80	1,51 12,30	12,30 100,00
10	montmorillonite Braňany NW Bohemia	7,07 58,50	0,93 7,70	2,49 20,60	1,28 10,60	0,32 2,60	12,09 100,00

determine the tetrahedron. If these four points represent silicates, the nex point also representing a silicate with the same representation of constituents should lie in the same tetrahedron in the case it belongs to the same group of silicates. We shall show on an example whether this assumption is correct.

From table 5 the silicates 2, 5, 7, 9 were taken, which determine the tetrahedron S_4 of superplane R_3. It is necessary to determine whether the silicate 6 (table 5) belongs to the same group of silicates.

Ranging is determined by examination whether the straight line R_1 drawn through point 6 and through one of the points of superplane R_3, e. g. 2, intersects plane R_2, determined by the points 5, 7, 9 (also in not proper point). If it intersects, the point 6 lies in R_3 (2, 3, 7, 9). The question is here the solution of the point of intersection of straight line R_1 with superplane R_3.

In fig. 6 projections of points 2, 5, 6, 7, 9 in R_4 are made in the known way

Table 6

No.	Mineral locality	Tetrahedrical coordination of ions		Octohedrical coordination of ions			Σ
		Si^{4+}	Al^{3+}	Al^{3+}	Fe^{3+}	Mg^{2+}	
11	nontronite (theor. const.)	7,34 61,2	0.66 5.5	— —	4,0 33,3	— —	12,00 100,00
12	nontronite Szekes-Fejer-var, Hungary	6,90 56,80	1,10 9.00	0,14 1,20	4,00 33,00	— —	12,14 100,00
13	nontronite Spokane Washington, USA	6,92 57.3	1,08 8.9	0,02 0,10	3,84 31,80	0,24 1.90	12,10 100.00
14	nontronite Spokane Washington, USA	7,00 57,9	1,00 8.30	0,12 0,90	3,84 31,80	0,14 1,10	12,10 100,00
15	nontronite Santa Rita N. Mexico	7,00 57,80	1,00 8.30	0,22 1,80	3,82 31,50	0,08 0,60	12,12 100,00
16	nontronite Nontron-Dordogne, France	7,44 62,00	0.56 4.70	0,16 1,30	3,68 30,70	0,16 1,30	12,00 100,00
17	nontronite Staryj Krym USSR	6,90 56,50	1,10 9,00	0,74 6,00	3,24 26,50	0,24 2,00	12,22 100,00
18	nontronite Staryj Krym USSR	7,54 63,10	0,46 3,80	1,38 11,50	2,52 21,0	0,06 0,60	11,96 100,00
19	nontronite Chevy Chase Madagaskar	6,94 57,30	1,06 8,70	2,04 16,80	2,08 17,20	— —	12,12 100,00
20	nontronite Petrovsk USSR	7,48 62,40	0,52 4,30	2,20 18,30	1,66 13,80	0,14 1,20	12,00 100,00

and for practical reasons transformation on axes y, u (20 y, 2 u) was carried out so that we carry on these axes complements of coordinates (components) only. We find four projections of the straight line q ($q_1 = 2_1 6_1$, $q_2 = 2_2 6_2$, $q_3 = 2_3 6_3$, $q_4 = 2_4 6_4$). We put through straight line $q = 6\ 2$ and $q_1 = 6_1 2_1$ the superplane R_3, which intersects plane R_2 (5, 7, 9) in straight line l, its first projection is $l_1 = q_1$. Finding of the second, third and fourth projection of straight line l as joints of projections of intersection points, e. g. l_1 and of straight lines $5_1\ 7_1$ or $7_1\ 9_1$ of plane R_2 of superplane R_3 is seen in fig. 6. The second projections $q_2\ l_2$ of straight lines q, l intersect in point Q_2, the third projections in point Q_3, the fourth projections in point Q_4. The first projection Q_1 of intersection point Q lies on the ordinate and on $q_1 = l_1$.

If the four projections Q_1, Q_2, Q_3, Q_4 of intersection point Q of straight lines q, l are peaks of a rectangle, its four sides are parallel with the axes x, y, z, u,

Table 7

No	Mineral Locality	Tetrahedral coordination of ions		Octahedral coordination of ions			Σ
		Si^{4+}	Al^{3+}	Al^{3+}	Fe^{3+}	Mg^{2+}	
21	talc (theor. const.)	8,00 57,20	— —	— —	— —	6,00 42,8	14,00 100,00
22	saponite Krugersdorf Transvaal	7,23 50,70	0,71 4,90	— —	0,06 0,40	6,32 44,00	14,32 100,00
23	saponite (theor. const.)	7,34 52,40	0,66 4,70	— —	— —	6,00 42,90	14,00 100,00
24	saponite Allt Ribhein Sweden	7,00 49,10	1,00 7,00	0,4 2,8	0,08 0,50	5,81 40,60	14,29 100,00
25	saponite Milford, Utah	7,49 53,60	0,51 3,70	0,17 1,20	0,03 0,20	5,75 41,30	13,95 100,00
26	saponite Cáslav	6,32 47,00	1,68 12,50	0,19 1,40	0,42 3,10	4,84 36,00	13,45 100,00

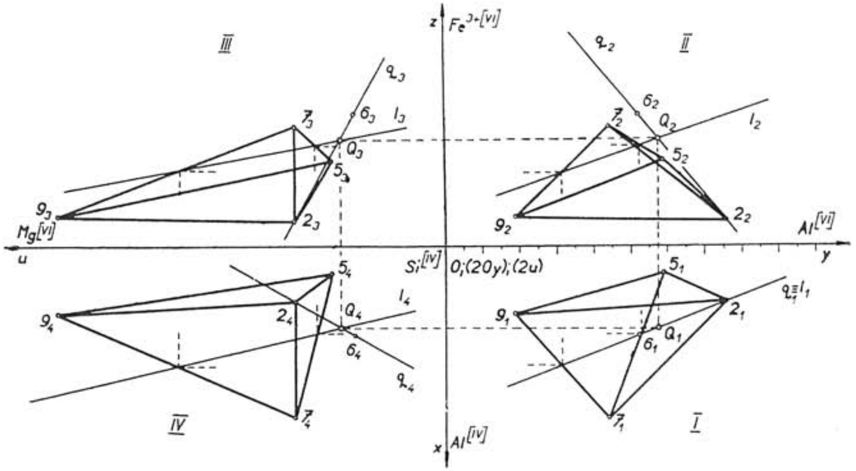

Fig. 6. Ranging of silicate in the supposed group of silicates.

straight line $q = 2\ 6$ intersects then plane R_2 (5, 7, 9) of superplane R_3 (2, 5, 7, 9) in point Q (all subspaces of four-dimensional space R_4), thus the point Q belongs to the superplane R_3 and the silicates represented by points 2, 5, 7, 9.

We remark that the condition expressed about the rectangle is to understand in a sense that it can have certain small deviation caused by less accuracy of analyses or calculations or also by graphic inaccuracy of solution.

Table 8

No.	Mineral locality	Tetrahedral coordination of ions		Octohedral coordination of ions			Σ
		Si^{4+}	Al^{3+}	Al^{3+}	Fe^{3+}	Mg^{2+}	
27	hydromuscovite B. Štiavnica ČSSR	5,9 49.20	2,1 17,5	3,85 32,10	0,05 0,40	0,10 0.80	12.00 100,00
28	hydromuscovite Ogofan Wales	6,0 51,5	2,0 17,2	3,53 30,30	0,04 0,03	0,10 0,70	11,67 100,00
29	muscovite (theor. const.)	6,00 50,00	2,00 16,7	4,00 33,30	— —	— —	12,00 100,00
30	hydromuscovite Nagybörzöny Hungary	6,25 53,0	1.75 14,80	3,55 30,20	0,10 0,80	0,15 1,20	11,80 100,00
31	illite (theor. const.)	6,5 54,2	1,50 12,50	4,00 33,30	— —	— —	12,00 100,00
32	illite Fithien Illinois, USA	6,81 56,60	1,19 9,90	2,79 23,20	0,68 5,70	0,55 4,60	12,03 100,00
33	beidellite Black-Jack USA	6,92 57,5	1,08 8,90	3,92 32,6	0,08 0,70	0,04 0,30	12,04 100,00
34	Veľká Kopan Transcarpathian USSR	7,08 58,60	0,92 7,60	3,23 16,80	0,66 5,40	0,20 1,60	12,09 100,00
35	beidellite Beidell Colorado, USA	7,16 60,60	0,84 7,00	2,78 23,30	1,00 8,40	0,16 1,30	11,94 100,00
36	beidellite (theor. const.)	7,34 61,20	0,66 5,50	4,00 33,00	— —	— —	12,00 100,00

We are going to show another, simpler way of ascertaining the group silicate belongs to. We choose a „pentastric" coordinal system in R_4 [essentially a special case of vectorial projecting in R_4 with employing of isoscelles trapezium, let us say A C E D B, where we considered point B (fig. 7) as the origin of coordinal system and the axes of coordinal system will be BA, BC, BD, BE] (J. Klimčík 1966).

On the axes BA and BC we carry the abscisses a, c, and we find the projection $M_{1,2}$ of point M. We draw through point $M_{1,2}$ a parallel with join DE and carry the abscissa $d = M_{1,2}M_3$ over in corresponding sense a $e = M_{1,2}M_4$. The coordinate b lies on the base AC and we determine it easily because $a+b+c+d = 100$ ($AC = 100$ units).

If we carry the coordinates d and e over from axes BA and BC (fig. 7), we reach advantageous construction as well as clearness of projections of point M.

In the same wey we construct projections of points 2, 5, 7, 9 (tab. 5)

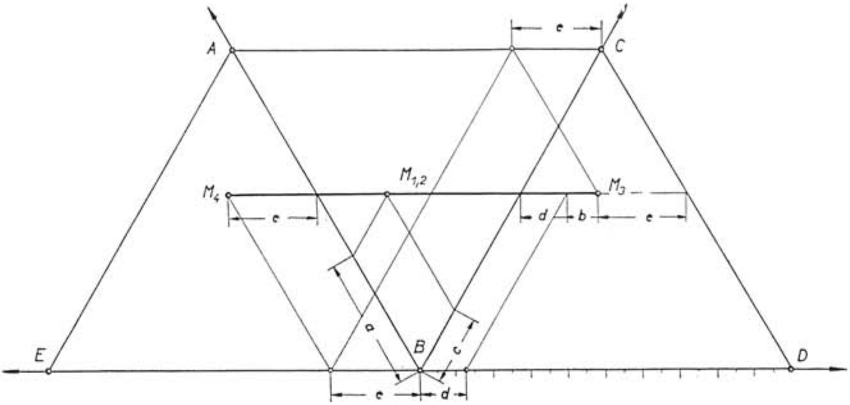

Fig. 7. Presentation of point in vectorial projection R_4 with employing of pentasteric coordinal system.

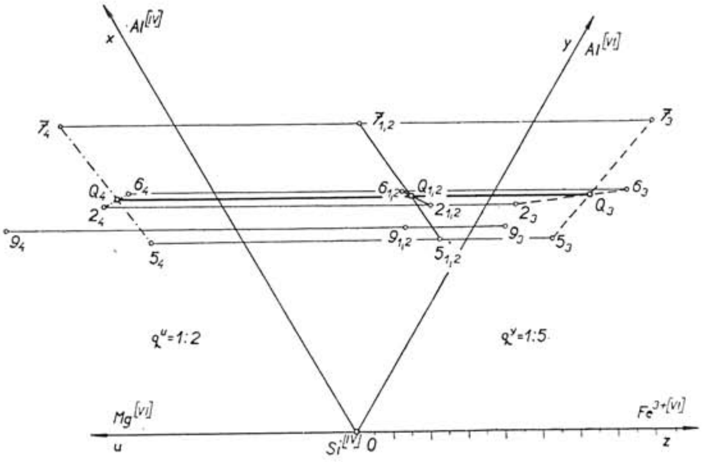

Fig. 8. Determination of silicate in the corresponding silicate group.

determining superplane R_3 and we ascertain belonging of point 6 to R_3. It is to remark that for practical reason the coordinates of all points are on axes y, u carried over in shortening ratio $q^y = 1:5$, $q^u = 1:2$. The solution of the point of intersection of straight line 2 6 with plane (5, 7, 9) in vectorial projecting R_4 chosen will be simplified from the graphic aspect (fig. 8). It is sufficient to find the point of intersection of straight line 2 6 with straight line 5 7 of plane R_2. The projections $Q_{1,2}$, Q_3,Q_4 of point of intersection Q lie on one straight line parallel to u or z, what confirms incidence of point 6 with superplane R_3. We conclude that silicate 6 belongs to the group of silicates represented by silicates 2, 5, 7, 9.

This second way of determination of the group silicate belongs to is more advantageous because we obtain here a diagram which is easy to construct. As to the study of relations of silicates or of relations of their components the foregoing way of presentation is more suitable and we come to conclusions analogous to those of H. E. Boeke (1916) in determination of tourmaline.

Conclusion

The projections of individual points present crystallochemical formulas of halloysite minerals from known classical localities and from localities in eastern Slovakia as compared with ideal halloysite and kaolinite. We can conclude from projections of individual points about their stechiometric interrelations in crystallochemical formulas.

We see that the projection of the point of ideal halloysite lies in the point of intersection D of the heights of tetrahedron (fig. 4). On the basis of the distribution of projections of points we may state that H_2O decreases in samples in the direction from A to the edge BC of tetrahedron so that kaolinite without adsorption water lies in the face BCD of tetrahedron. In a similar way we can read out the changes of the constituent of Si content in the direction from B to Ac and the changes of Al constituent in the direction from C to Ab. We see the changes of constituents of OH directly in terminal projections $1' \ldots 9'$ points $1 \ldots 9$, representing individual samples.

In this paper the graphic way of investigation of three-bedded silicates relations is shown and that in four-dimensional space R_4 with the subspaces R_0, R_1, R_2, R_3, in their representation crystallochemical were used. The application of this way of representation enables to distinguish groups of three-bedded silicates, also groups being very similar from the aspect of crystallochemistry. The possibility of graphic determination of the group certain three-bedded silicate belongs to also is indicated.

Translated by J. Pevný.

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