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The Quantitative Mineral Composition of Sedimentary Rocks: Calculation from Chemical Analyses and Assessment of Adequacy (MINLITH Computer Program)

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Abstract—The MINLITH program provides for calculating the first approximation mineral composition of sedimentary rocks and their metamorphic counterparts from the bulk chemical compositions. The method is universal and can be applied to most types of clastic, pelitic, and carbonate sedimentary rocks based on a limited set of minerals and their simplified compositions. The program comprises a great number of arithmetic operations making up an algorithm. Each operation solves the equations allocating the major oxides to possible (expected) normative minerals. The operation sequence is determined from empirical relationships based on the study of numerous reference samples. The accuracy of MINLITH calculations was statistically estimated from comparison with results of the high-precision study of modal mineral compositions. Uncertainty is commonly within a range of 5–15 rel % and attains 60–70 rel % if the mineral content is below 5 wt %. It is evident that the program is a rather simple, convenient, and useful tool for the approximate estimation of mineral compositions of sedimentary rocks for lithological purposes.

INTRODUCTION

The calculation of mineral composition of rocks from their bulk chemical composition is an efficient method for the genetic interpretation, comparative study, and systematics of rocks. The well-known CIPW system elaborated in the early 20th century is still applied to igneous petrology. Such methods were not popular in lithology, first of all, because the mineral composition in sedimentary rocks is much more complex and methods of its identification with a required accuracy were much later developed. The normative mineral composition is calculated with the MINLITH program on PC with a satisfactory accuracy, and the calculation is practically instantaneous for the clastic, pelitic, carbonate, and other rocks. Therefore, the MINLITH program allows the processing of large data arrays that are inaccessible for common physical methods (counting in thin sections, X-ray diffractometry, and others). Since contents of H_2O (in any form) and CO_2 are ignored in the program, it is also possible to estimate the primary mineral composition of metasedimentary rocks in order to elucidate ancient sedimentation environments. Examples of successful application of the program were reported in several publications (Aksamentova *et al.*, 2002; Rosen *et al.*, 1999, 2000, 2002; Zlobin *et al.*, 2002).

NORM CALCULATIONS: A BRIEF OVERVIEW

Interactive computer programs for calculation of the mineral composition of sedimentary rocks are proposed in several recent publications (Pactunc, 1998; Caritat *et al.*, 1994; Currie, 1991). However, these programs are based on the known compositions of modal minerals, and this makes the investigation too cumbersome. Several high-precision computing methods were proposed for pelites (Pearson, 1978; Kolka *et al.*, 1994; Laird and Dowdy, 1994; Merodio *et al.*, 1992), but their application requires X-ray diffraction data for the estimation of mineral contents. The SEDNORM program (Cohen and Ward, 1991; Ward and Taylor, 1996) uses the chemical composition of rocks for the calculation of mineral norms. However, this program requires the instrumental determination of compositions of variable phases, such as smectite, illite, chlorite, and others. If this information is lacking as in the case of metamorphic rocks, approximately nine degrees of freedom (mineral composition variants) are left in the calculation, and results turn out to be uncertain. Researchers have also proposed standardless methods, which do not require comparison with reference minerals observed in the rock, for the interpretation of XRD results. However, the expected phase compositions should be known beforehand in such programs. It is evident that these methods most likely serve as a supplement to common instrumental (physical) methods for the

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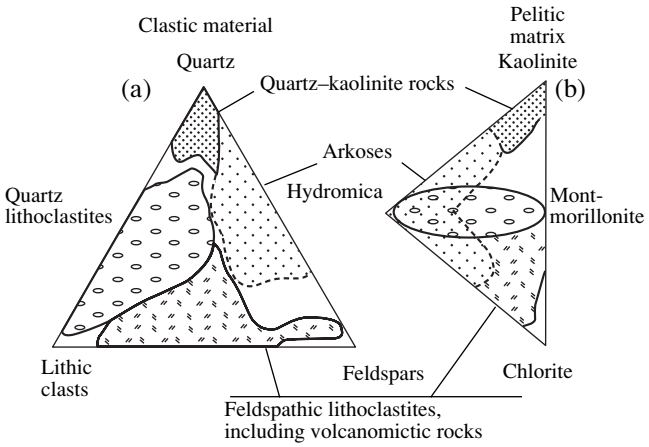

Fig. 1. (a) Families of terrigenous rocks vs. (b) prevailing clay minerals (modified after Kossovskaya and Shutov, 1971).

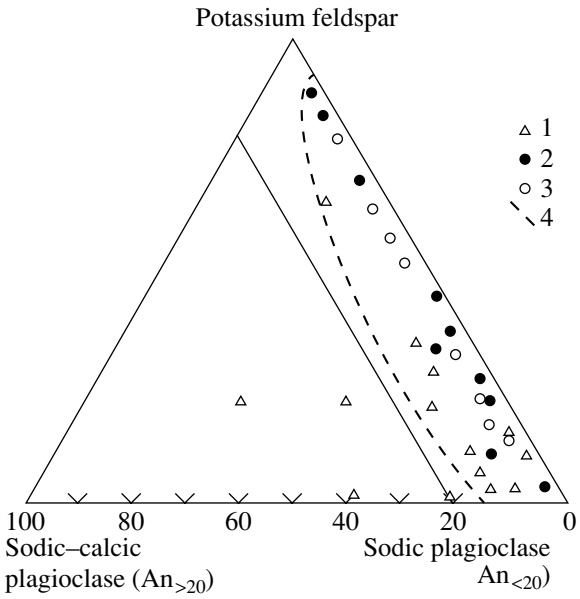

Fig. 2. Composition of feldspars in sandstone clasts (modified after Shutov, 1975). (1) Petrogenic complexes related to direct supply of clastic materials from acid, intermediate, and basic igneous rocks (each data point characterizes a series of samples of one age level); (2) lithoclastogenic complexes; (3) aposaprogenic complexes related to erosion of weathered rocks; (4) prevailing composition domain.

determination of mineral composition rather than a universal tool for the study of sedimentary rocks. Some other methods applied to the high-precision quantitative mineralogical analysis of sedimentary rocks are mentioned below in the section devoted to assessment of the accuracy of norm calculations with the MINLITH program.

CHOICE OF NORMATIVE MINERALS

In order to calculate the normative composition of any sedimentary rock and compile the computation algorithm, we have to simplify the set of minerals and their compositions. Main problems arise with aluminosilicates, especially clay minerals that compose approximately 75% of sediments. The accepted systematics is shown in Fig. 1. Erosion products of weathering crust largely consist of kaolinite and quartz, whereas graywackes are mainly composed of feldspars, lithic clasts, and chlorite. The intermediate group comprises arkose, quartz–lithic clastic rocks, and so on with illite and smectite in addition to feldspars and lithic clasts. This list of components includes four clay minerals chosen for the norm calculation (kaolinite, illite, smectite, and chlorite) and other common minerals, such as feldspars, including plagioclase (albite and anorthite) and K-feldspar. Other components (dark-colored pyroxene, olivine, and amphibole) and rock fragments are out of the system owing to the absence of differences that would make it possible to discriminate the major oxides. This simplification is not serious if the calculation results are correctly interpreted. Thus, the proposed algorithm is restricted by seven aluminosilicate components (four clay minerals and three feldspars). The plagioclase composition was additionally simplified and accepted as An 20% commonly found in most clastic rocks (Fig. 2).

The theoretical kaolinite composition was accepted for the pelitic group. The accepted illite and montmorillonite (smectite) compositions correspond to their authigenic varieties in natural rocks (Rosen and Nistratov, 1984).

The chlorite component of sedimentary rocks is characterized by an extremely wide compositional variation. Correlation between chlorite and host rock composition was established on the basis of bulk iron content (FeOtot = FeO + 0.9Fe_2O_3, wt %). Mole fractions of FeO, i.e., F = FeOtot/(FeOtot + MgO), mol % are approximately equal in chlorite and rock ($F_{CHL}/F_{rock} \approx 1$). The Al_2O_3 content shows two types of correlation between the chlorite and rock. When $F_{CHL} > 0.78$, the mole fraction of Al_2O_3 in chlorite, i.e., $A_{CHL} = 2Al_2O_3/(2Al_2O_3 + MgO + FeOtot)$, mol % is approximately equal to this parameter in rock (A_{rock}), where $Al_2O_3 = Al_2O_{3rock} - (Na_2O + K_2O)_{rock}$. If $F_{CHL} < 0.78$, $A_{CHL}/A_{rock} \sim 0.5$ (Fig. 3). Average chemical compositions of modal chlorites were estimated for common rock types within the F range of 0.2–0.9, and the respective crystallochemical formulas were calculated on the basis of 10 cations. Thus, a simplified petrochemical systematics of chlorites from sedimentary rocks was presented as a combination of four end members (greenalite, chamosite, amesite, and serpentine) without regard for their crystal chemistry (Fig. 4).

The petrochemical simplification serves as a basis for the general formula of chlorite accepted in the MIN-

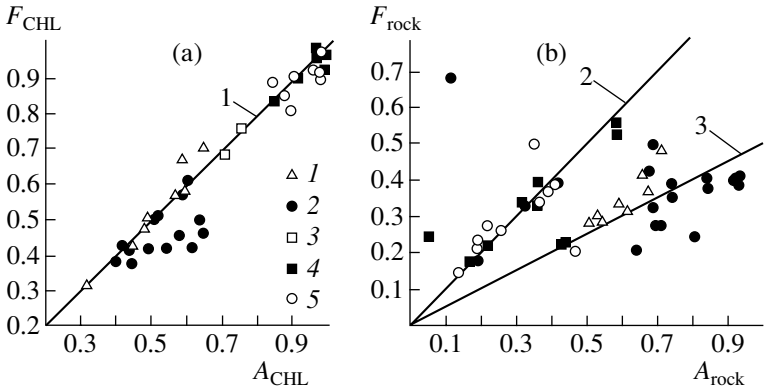

Fig. 3. (a) *F* vs. (b) *A* relationship in chlorites and host rocks. F = FeOtot/(FeOtot + MgO); $A = 2Al_2O_3/(2Al_2O_3 + MgO + FeOtot)$, where $Al_2O_3 = Al_2O_{3rock} - (Na_2O + K_2O)_{rock}$, mol %. (1) Graywacke; (2) mudstone; (3) Fe–Al nodule; (4) siderite; (5) brown iron ore.

LITH program: $k1MgO \cdot k2FeO \cdot k3Al_2O_3 \cdot k4SiO_2 \cdot 4H_2O$, where k1 + k2 + k3 + k4 = 10. Equations for the calculation of coefficients k1–k4 are given in Table 1. If the calculated chlorite composition is compared with other analytical results, the program yields a standard formula $(Me^{2+})_4(Me^{3+})_2(Al, Si)_4O_{10}(OH)_8$. All the formulas used are shown in Table 2.

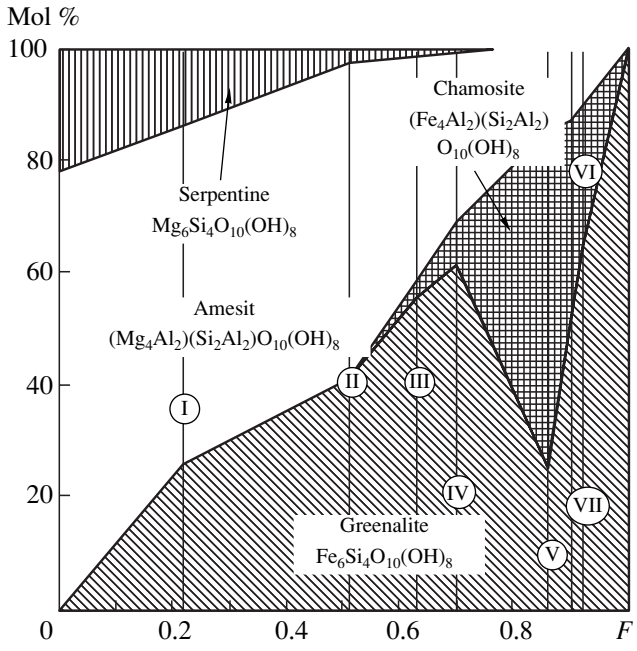

Fig. 4. End members of chlorite from sedimentary rocks vs. *F* value. Average composition of chlorites in: (I) carbonate rocks and evaporites, (II) graywackes, (III) polymictic and quartz sandstones, (IV) clays, (V) allites and ferriallites, (VI) siderites and ferruginous carbonate rocks, (VII) brown iron ore. Formulas were calculated for 10 cations irrespective of crystallochemical structure.

RELATIONSHIPS BETWEEN NORMS AND MODES

When comparing XRD data with normative compositions, we should keep in mind that the normative illite corresponds to the group of nonexpanding clay minerals, including the authigenic illite, detrital (relict) dioctahedral K-mica (1Md-type with a potassium deficiency balanced by the H_3O^- group), and a small amount of mixed-layer phases. The normative montmorillonite comprises the montmorillonite, other smectites, and mixed-layer phases consisting of illite–smectite intercalations that include partly ordered modifications with 10–20% expanding layers or disordered modifications with more than 40% expanding layers. The latter modification can also partly enter the normative chlorite.

Considerable limitations in interpretation are caused by the fact that the normative compositions correspond to mature sediments that underwent a long-term transfer, redeposition, and diagenetic alteration. As a result, fragments of volcanic rocks and dark-colored minerals (olivine, pyroxene, amphibole, and others) are completely decomposed or replaced by minerals of mature sedimentary rocks. If dark-colored minerals or fragments of basic igneous rocks remain in a sedimentary rock, its normative composition becomes enriched in chlorite, as it takes place in graywackes where the mafic fragments are replaced by Fe–Mg layer silicates. The quartz–feldspar normative composition, which is doped with illite and montmorillonite replacing the modal mica and amphibole, respectively, is typical of felsic (granitic) rocks. A similar composition is typical of silicic volcanic glass. Various structural classifications of sedimentary rocks based on the proportions of silica minerals and lithic clasts are inadequate for normative compositions, because they are insensitive to these proportions. At the same time, the normative compositions are indispensable for the comparison and correlation of large

Table 1. A system of equations for the calculation of coefficients k1–k4 in the chlorite formula $k1MgO \cdot k2FeO \cdot k3Al_2O_3 \cdot k4SiO_2 \cdot 4H_2O$

No.	Parameter[1]	Equation				Calculated molecular weight
		k1	k2	k3	k4	
1	$0 \le F \le 0.21$	$-5.18F + 4.42$	$4.09F$	$(0.41F + 3.16)/2$	$10-(k1 + k2 + 2k3)$	$126.89F + 551.81$
2	$0.21 \le F < 0.51$	$-2.96F + 3.93$	$5.66F - 0.34$	$(-2.69F + 3.66)/2$	$10-(k1 + k2 + 2k3)$	$126.89F + 551.81$
3	$0.51 \le F \le 0.69$	$-5.32F + 5.13$	$2.54F + 1.24$	$(3.46F + 0.53)/2$	$10-(k1 + k2 + 2k3)$	$126.89F + 551.81$
4	$0.69 < F \le 0.87$[2]	$-5.32F + 5.13$	$2.54F + 1.24$	$(3.46F + 0.53)/2$	$10-(k1 + k2 + 2k3)$	$126.89F + 551.81$
4a	$0.40 < A < 0.47$	$-12A + 6.2$	$2.54F + 1.24$	$(3.46F + 0.53)/2$	$10-(k1 + k2 + 2k3)$	$126.89F + 551.81$
4b	$A \ge 0.47$	0.56	$2.54F + 1.24$	$(3.46F + 0.53)/2$	$10-(k1 + k2 + 2k3)$	$126.89F + 551.81$
5	$0.87 < F < 1$	$-4F + 4$	$18.36F - 12.36$	$(-25F + 25)/2$	$10-(k1 + k2 + 2k3)$	$561.42F + 182.12$

Notes: [1] $F = FeO/(FeO + MgO)$; $A = 2Al_2O_3/(2Al_2O_3 + MgO + FeO)$, mol %.
[2] In the range of $0.69 < F \le 0.87$ and high-Al rocks (A > 0.40), coefficient k1 is calculated from Eqs. 4a or 4b depending on the *A* value.

stratigraphic units characterized by a great number of chemical analyses.

The normative mineral composition of metasedimentary rocks can be regarded as an approximation to the modal protolith composition. In sedimentary rocks of uncertain origin, the normative minerals can simply be designated as petrochemical components in the following way: (Q) silicic component, e.g., in chert; (AB, OR) alkali–alumina component, e.g., in anorthoclase or zeolites; (ILL, MM) alkali Mg–Fe component; and (CHL) Mg–Fe–Al component.

The occurrence of MM and Na–Mg–Fe–Al components may indicate a presence of mixed-layer minerals. The assemblage of normative ILL, MM, and CHL, as a whole, may correspond to various mixed-layer phases. However, their total content would not probably exceed the sum of these normative components.

THE MINLITH ALGORITHM

The procedure allocates the oxide-to-mineral transformation in three sequential stages and a few substages making up the program. The results are expressed in wt %. The algorithm comprising about 700 operations includes the direct calculation of each mineral from the respective (critical) major elements (except volatile components) and the subsequent control from contents of other rock-forming elements. A deficiency in any of these elements returns the program to the preceding stage, and the allocation of elements to other minerals is resumed according to empirical relationships established in standards (600 reference samples taken from the literature). The obtained mineral composition is a unique result of arithmetic calculations (Rosen *et al.*, 2000).

The principal computation stages are shown in Fig. 5.

(1) The computation of accessory and subsidiary components on the stoichiometry basis of apatite (P), pyrite (S_{pyr}), gypsum (SO_3), and fluorite (F). Carbon (C_{org}) and rutile (TiO_2) are directly incorporated into the final results.

(2) The computation of aluminosilicates and gibbsite from the alumina allocation to the respective normative minerals according to the known Na, K, Ca, Mg, Fe, and Si contents (Table 3). However, the number of elements used for the calculation of mineral balance (Na, K, Ca, Mg, Fe, and Si), i.e., the number of equations is insufficient for a unique solution (the number of minerals or unknowns is more than the number of equations). Therefore, the program uses additional empirical equations based on standards, i.e., 600 published quantitative mineral analyses accompanied by the bulk chemical compositions. These equations allocate Al_2O_3 contents to the respective Al-bearing minerals. Kaolinite and feldspars are eliminated from the calculation at the very low or, on the contrary, very high Al_2O_3 contents, respectively.

(3) The amounts of Si, Fe, Mg, and Mn remained after the first and second stages are allocated to silicates, oxides, and carbonates according to the excess or deficiency of remaining Ca. The Ca residue equal to 250 units of oxide molecular quantities (1.40 wt % CaO) is an identification level of contents that governs the following operations. If $Ca^{n+2} \le 250$, the subsequent computation of Fe and Mn distribution is performed in oxide form. However, if $Ca^{n+2} > 250$, the carbonate forms are calculated (Table 4).

Each calculation procedure yields a residue, which is consumed at the next step. The oxide excess, which

Table 2. Formulas of minerals used in the MINLITH program

Abbreviation	Mineral	Formula	Molecular weight[1]
AB	Albite	$Na_2O \cdot Al_2O_3 \cdot 6SiO_2$	524.482
AN	Anorthite	$CaO \cdot Al_2O_3 \cdot 2SiO_2$	278.22
ANK	Ankerite	$CaO \cdot FeO \cdot 2CO_2$	215.952
AP	Apatite	$3CaO \cdot P_2O_5 + 1/3(CaF_2)$	336.21
CC	Calcite	$CaO \cdot CO_2$	100.091
CHL	Chlorite	$k1MgO \cdot k2FeO \cdot k3Al_2O_3 \cdot k4SiO_2 \cdot 4H_2O$[2]	555.81–743.54
C_{org}	Carbon	C	12.011
DL	Dolomite	$CaO \cdot MgO \cdot 2CO_2$	184.422
FL	Fluorite	CaF_2	78.08
GB	Gibbsite	$Al_2O_3 \cdot 3H_2O$	156.08
GT	Goethite	$Fe_2O_3 \cdot H_2O$	177.716
GY	Gypsum	$CaO \cdot SO_3 \cdot 2H_2O$	172.178
HL	Halite	$Na_2 \cdot 2Cl$	116.896
ILL	Illite	$2K_2O \cdot MgO \cdot FeO \cdot 6.5Al_2O_3 \cdot 16SiO_2 \cdot 5H_2O$	2014.75
KN	Kaolinite	$Al_2O_3 \cdot 2SiO_2 \cdot 2H_2O$	258.172
MM	Montmorillonite	$Na_2O \cdot 2MgO \cdot 5Al_2O_3 \cdot 24SiO_2 \cdot 6H_2O$	2202.60
MST	Magnesite	$MgO \cdot CO_2$	84.331
OR	Orthoclase	$K_2O \cdot Al_2O_3 \cdot 6SiO_2$	556.70
PR	Pyrite	FeS_2	119.982
PRL	Pyrolusite	MnO_2	86.94
Q	Quartz	SiO_2	60.09
RCH	Rhodochrosite	$MnO \cdot CO_2$	114.951
RT	Rutile	TiO_2	79.90
SD	Siderite	$FeO \cdot CO_2$	115.861
SRP	Serpentine	$3MgO \cdot 2SiO_2 \cdot 2H_2O$	277.172

Notes: [1] Molecular and atomic weights used in calculations (Avidon, 1976; Rosen *et al.*, 1982): SiO_2 60.09; TiO_2 79.90; Al_2O_3 101.96; FeO 71.85; MnO 70.94; MgO 40.32; CaO 56.08; Na_2O 61.982; K_2O 94.20; P_2O_5 141.95; S 32.066; C 12.011; SO_3 80.066; F 19.00; Cl 35.457.
[2] See Table 1 for calculations of factors k1–k4.

did not enter the calculated minerals, is converted into the respective simple minerals, and this is the end of computation expressed in molecular quantities. At the subsequent stage, the molecular quantities of aluminosilicates, carbonates, silicates, and oxides (recalculated into wt %) are corrected to 100%. Computation with the MINLITH program is completed at this stage.

Contents of H_2O (in any form) and CO_2 are ignored in calculations. They can be estimated from the normative mineral composition using the above-mentioned formulas. These estimates are commonly consistent with volatile element contents recorded in chemical analyses of unmetamorphosed rocks.

ACCURACY OF RESULTS AND EXAMPLE OF CALCULATIONS

Statistical Comparison of Normative and Modal Compositions

The degree of compliance between norms and modes is a key point in elaboration of the universal method applicable to all sedimentary rocks. Any method of the quantitative study of chemical substances is characterized by two principal parameters: (1) accuracy (reliability) and (2) precision (reproducibility). Methods of analytical chemistry, petrographic methods, and X-ray diffractometry are characterized by

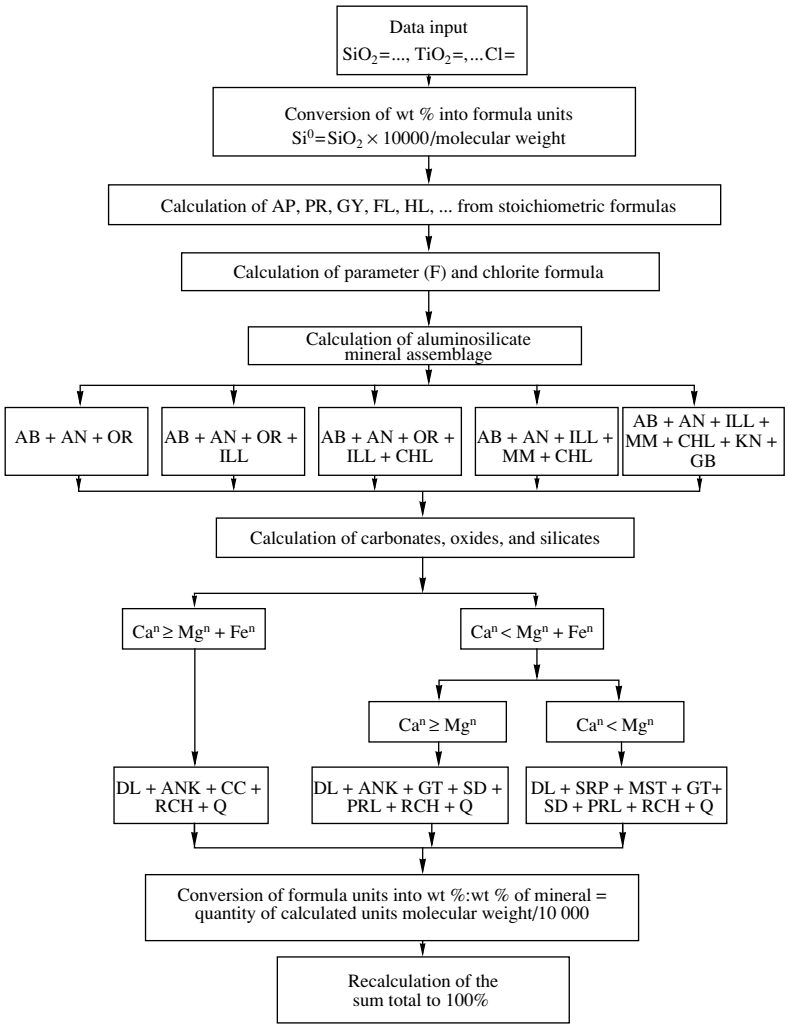

Fig. 5. Block scheme of the MINLITH program.

specific accuracy limits affecting the results of normative mineral calculations. For example, insignificant errors in the reproducibility of chemical analysis in the case of alkali metal contents give rise to large errors in the calculated mineral contents, which can attain n. 10% (Shaw, 1964).

The correlation between normative and modal compositions is typically better than 0.7 (Fig. 6). The accuracy of normative mineral content determination (irrespective of the bulk content) can be assessed by the root-mean-square error or variation coefficient (*Vd*) expressed in relative percentages according to the following equation (Nalimov, 1960; Aksamentova, 1975):

$$Vd = \sqrt{\frac{\sum_{i=1}^{i=n}\left(\frac{d_i}{\bar{x}_i}\times 100\right)^2}{2n}},$$

where n is the number of parallel normative and modal values (wt %), $d_i = |x_{i1} - x_{i2}|$ is the absolute difference between normative and modal values for the ith pair and $\bar{x}_i = (x_{i1} - x_{i2})/2$ is the average value. We used the modal mineral compositions and bulk chemical compositions of 115 samples from the Australian Platform (Mumme *et al.*, 1996), Russian Platform (Ronov *et al.*, 1972, 1990), and Siberian Platform (Rosen *et al.*, 1999). The correlation results are presented in Fig. 7. The discrepancy between normative and modal contents is the lowest (*Vd* = ±5–15 rel % with a maximum of ±40–50 rel % for OR or FSP) for most minerals if the norms are compared with the most reliable modal compositions of platformal sedimentary rocks (Mumme *et al.*, 1996; Ronov *et al.*, 1972, 1990; Rosen *et al.*, 1999). A good agreement between norms and modes was established for rocks from the Australian Platform (Mumme *et al.*, 1996). In this case, *Vd* generally varies from ±5 to 14 rel % and reaches 50–60 rel % for feldspars. A satisfactory precision (*Vd* = 13–40 rel %) was obtained for most components in rocks from the Russian Platform analyzed at the Geological Research

Table 3. Algorithm for the calculation of aluminosilicate minerals

Stage 1. Calculated alumina fractions depending on Me_2O and MeO contents in mineral formula

Alumina fraction in minerals	Me_2O, MeO[1]
Al_{AB}	Na_{AB}
Al_{OR}	K_{OR}
Al_{AN}	0.2 Na_{AB}[2]
Al_{ILL}	3.25 K_{ILL}
Al_{MM}	5 Na_{MM}
Al_{CHL}	$[Mg^0-(Mg_{ILL} \pm Mg_{MM}) \times k3]/k1$

Stage 2. Variable mineral assemblages corresponding to gradually increasing alumina content in the bulk composition (Al^0)

Gradation of increase in Al_2O_3	Allocation of initial alumina (Al^0) to normative minerals
1	$Al_{AB} + Al_{OR} \le Al^0 \le Al_{AB} + Al_{AN} + Al_{OR}$
2	$Al_{AB} + Al_{AN} + Al_{OR} < Al^0 \le Al_{AB} + Al_{AN} + + Al_{ILL} + Al_{OR}$
3	$Al_{AB} + Al_{AN} + Al_{ILL} + Al_{OR} < Al^0 \le Al_{AB} + + Al_{AN} + Al_{ILL} + Al_{OR} + Al_{CHL}$
4	$Al_{AB} + Al_{AN} + Al_{ILL} + Al_{CHL} < Al^0 \le Al_{MM} + + Al_{ILL} + Al_{CHL}$
5	$Al_{MM} + Al_{ILL} + Al_{CHL} < Al^0 \le Al_{MM} + Al_{ILL} + + Al_{CHL} + Al_{KN} + Al_{GB}$

Stage 3. Determination of alumina fractions in aluminosilicates based on allocation equations

Gradation of increase in Al_2O_3	Alumina fractions (in aluminosilicates) used for calculations[3]	Equations of alumina fraction allocation between alumosilicates	Control[4]
1	$Al_{AB} = Na^0$; $Al_{OR} = K^0$; $Al_{AN} = 0.2Na^0$	(AB + OR(AN)): $Al^0 = Al_{AB} + Al_{OR} \pm A1^5_{AN}$	Ca^n, Si^n
2	$Al_{AB} = Na^0$; $Al_{AN} = 0.2Na^0$; $Al_{OR} = K_{OR}$; $Al_{ILL} = 3.25K_{ILL}$	(OR + ILL): $K^0 = K_{OR} + K_{ILL}$; $Al^0 = Al_{AB} + Al_{AN} + Al_{OR} + Al_{ILL}$	Ca^n, Mg^0, Fe^1, Si^n
3	$Al_{AB} = Na_0$; $Al_{AN} = 0.2Na^0$; $Al_{ILL} = 3.25K_{ILL}$; $Al_{OR} = K_{OR}$; $Al_{CHL} = (Mg^0 - Mg_{ILL}) \times k3/k1$	(OR + ILL + CHL): $K^0 = K_{OR} + K_{ILL}$; $Na^0 = Na_{AB}$; $Al^0 = Al_{AB} + Al_{AN} + Al_{OR} + Al_{ILL} + Al_{CHL}$; $Mg_0 = Mg_{ILL} + Mg_{CHL}$	Ca^n, Fe^1, Si^n
4	$Al_{AB} = Na_{AB}$; $Al_{AN} = 0.2\ Na_{AB}$; $Al_{ILL} = 3.25\ K^0$; $Al_{MM} = 5\ Na_{MM}$; $Al_{CHL} = (Mg^0 - Mg_{ILL} + Mg_{MM}) \times k3/k1$	(AB + AN + MM + CHL): $K^0 = K_{ILL}$; $Na^0 = Na_{AB} + Na_{MM}$; $Al^0 = Al_{AB} + Al_{AN} + Al_{ILL} + Al_{MM} + Al_{CHL}$; $Al_{AN} = 0.2\ Na_{AB}$; $Mg^0 = Mg_{ILL} + Mg_{MM} + Mg_{CHL}$	Ca^n, Fe^1, Si^n
5	$Al_{AB} = Na_{AB}$; $Al_{AN} = 0.2\ Na_{AB}$; $Al_{ILL} = 3.25\ K_{ILL}$; $Al_{MM} = 5\ Na_{MM}$; $Al_{CHL} = (Mg^0 - Mg_{ILL} + Mg_{MM}) \times k3/k1$; $Al_{KN} = 0.5\ Si_{KN}$; Al_{GB}	(AB + AN + MM + CHL): $K^0 = K_{ILL}$; $Na^0 = Na_{AB} + Na_{MM}$; $Al^0 = Al_{AB} + Al_{AN} + Al_{ILL} + Al_{MM} + Al_{CHL} + Al_{KN} \pm \pm Al_{GB}$ $Al_{AN} = 0.2\ Na_{AB}$; $Al_{KN} = 0.5\ Si_{KN}$; $Mg^0 = Mg_{ILL} + Mg_{MM} + Mg_{CHL}$; $Si^0 = Si_{AB} + Si_{AN} + Si_{OR} + Si_{ILL} + Si_{MM} + Si_{CHL} + + Si_{KN}$	Al^0, Fe^1

Notes: Contents of all elements are expressed in molecular quantities of oxides.

[1] Me_2O and MeO are molecular quantities of Na_2O, K_2O, and MgO denoted as Na, K, and Mg, respectively, in normative minerals AB, OR, ILL, MM, and CHL (see Table 1 for abbreviations).

[2] According to the accepted conditions and formulas, Al_{AN} is calculated as 20% of albite based on the Na content; Al_{CHL} with respective formula coefficients k1 and k2 is defined as alumina residue in montmorillonite and illite, where $Mg_{ILL} = 0.5K_{ILL}$ and $Mg_{MM} = 0.2Na_{MM}$.

[3] Na^0, Na^1 and Na^n are oxide concentrations in the bulk chemical composition (^{0}), in residue left after the first calculation (^{1}), and after *n* number of preceding calculations.

[4] It is verified at this stage, whether the amount of other elements is sufficient for the formation of the specified minerals. If this condition is not fulfilled, the program returns to the preceding stage and uses other components for the solution.

[5] AN is calculated from alumina residue left after the calculation of all other minerals when the condition $Al^0 \ge Al_{AB} + Al_{ILL} + Al_{OR} + Al_{MM} + Al_{CHL} + Al_{KN}$ is fulfilled.

Table 4. Algorithm for the calculation of carbonates, silicates, and oxides

Stage 1. Selection of minerals and residual oxides

Mineral	Residual oxide
DL	Mg^n, Mg^{n+1}, Ca^n
CC	Ca^n
ANK	Fe^n, Ca^{n+1}
RCH	Mn^0
SD	Fe^n, Fe^{n+1}
PRL	Mn^0
GT	$Fe^n/2$, $Fe^{n+2}/2$[1]
SRP	$Si^n/2$, $Mg^{n+1}/3$
MST	Mg^{n+1}, $Mg^{n+1}–3Mg_{SRP}$
Q	Si^n

Stage 2. Selection of relationships between residual oxides as guides for the subsequent computation

Type	Relationship
I.	$Ca^n \geq Mg^n + Fe^n$
II.	$Ca^n < Mg^n + Fe^n$
1.	$Ca^n \geq Mg^n$
II. 1a	$Ca^{n+2} \leq 250$
II. 1b	$Ca^{n+2} > 250$
2.	$Ca^n < Mg^n$
II. 2a	$Si^n \geq 2/3(Mg^n–Ca^n)$
II. 2b	$0 < Si^n < 2/3(Mg^n–Ca^n)$
II. 2c	$Si^n = 0$

Stage 3. Calculation of normative carbonates, silicates, and oxides

Relationships of residual oxides	Dolomite	Magnesite, ankerite, and serpentine	Calcite, siderite, and goethite	Rhodochrosite, pyrolusite, and quartz
	1[2]	2	3	4
I	$Mg^n + Ca^{n+1}_{(=Mg^n)} \longrightarrow$ DL[3]	$Ca^{n+1}_{(=Fe^n)} + Fe^n \longrightarrow$ ANK	$Ca^{n+3}_{(=Ca^n–Ca^{n+1}–Ca^{n+2})} \longrightarrow$ CC	$Mn^0 \longrightarrow$ RCH, $Si^n \longrightarrow$ Q
II. 1a	$Mg^n + Ca^{n+1}_{(=Mg^n)} \longrightarrow$ DL	$Ca^{n+2}_{(=Ca^n–Ca^{n+1})} + Fe^{n+1}_{(=Ca^{n+2})} \longrightarrow$ ANK	$Fe^{n+2}_{(=Fe^n–Fe^{n+1})} \longrightarrow$ GT	$Mn^0 \longrightarrow$ PRL, $Si^n \longrightarrow$ Q
II. 1b	$Mg^n + Ca^{n+1}_{(=Mg^n)} \longrightarrow$ DL	$Ca^{n+2}_{(=Ca^n–Ca^{n+1})} + Fe^{n+1}_{(=Ca^{n+2})} \longrightarrow$ ANK	$Fe^{n+2}_{(=Fe^n–Fe^{n+1})} \longrightarrow$ SD	$Mn^0 \longrightarrow$ RCH, $Si^n \longrightarrow$ Q
II. 2a	$Ca^n + Mg^{n+1}_{(=Ca^n)} \longrightarrow$ DL	$Mg^{n+2}_{(=Mg^n–Mg^{n+1})} + Si_{(=2/3Mg^{n+2})} \longrightarrow$ SRP	$Fe^n \longrightarrow$ GT	$Mn^0 \longrightarrow$ PRL $Si^{n+2}_{(=Si^n–Si^{n+1})} \longrightarrow$ Q
II. 2b	$Ca^n + Mg^{n+1}_{(=Ca^n)} \longrightarrow$ DL	$Si^n + Mg^{n+2}_{(=1–1/2Si^n)} \longrightarrow$ SRP $Mg^{n+3}_{(=Mg^n–Mg^{n+1}–Mg^{n+2})} \longrightarrow$ MST	$Fe^n \longrightarrow$ GT	$Mn^0 \longrightarrow$ PRL $Si^{n+2}_{(=Si^n–Si^{n+1})} \longrightarrow$ Q
II. 2c	$Ca^n + Mg^{n+1}_{(=Ca^n)} \longrightarrow$ DL	$Mg^{n+2}_{(=Mg^n–Mg^{n+1})} \longrightarrow$ MST	$Fe^n \longrightarrow$ SD	$Mn^0 \longrightarrow$ RCH

Notes: Contents of all elements are expressed in molecular quantities of oxides.

Residual components remained after the calculation of aluminosilicates are computed (Table 3).

[1] Designations like Fe/2 are calculated formula units. For example, values used for recalculation to wt % are as follows: 1/2 Fe_2O_3 for goethite $Fe_2O_3 \cdot H_2O$, 1/3 MgO and 1/2 SiO_2 for serpentine $3MgO_2 \cdot 2SiO_2$, MgO for magnesite $MgO \cdot CO_2$, and so on.

[2] (1–4) Sequential operations in mineral calculation.

[3] Subscript (=Mg^n) related to Ca^{n+1} indicates that the Ca value equal to the molecular quantity of Mg^n is subtracted from the preceding Ca^n value with a formation of the next Ca^{n+1} value used in subsequent computations. Arrow denotes that both components make up dolomite. Calculated formula units of dolomite are similar (Mg^n or Ca^{n+1}) according to the formula $CaO \cdot MgO \cdot 2CO_2$. Other operations 1–4 are carried out in the similar manner according to the calculated formula units of Stage 1.

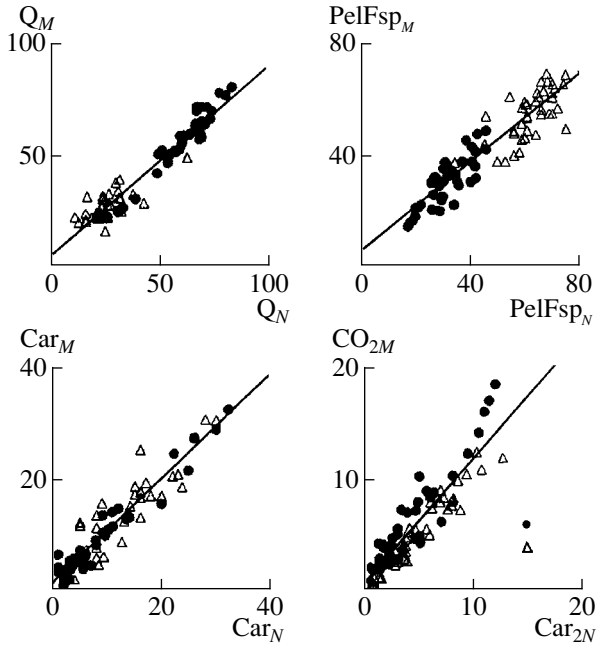

Fig. 6. Correlation of normative (N, this work) and modal (M) contents of mineral components. (1) Silty and sandy rocks (Ronov *et al.*, 1995); (2) pelitic rocks (Ronov *et al.*, 1990); (Car) sum of calcite, dolomite, ankerite, and rhodochrosite; (PelFsp) sum of Pel (illite, chlorite, montmorillonite, and kaolinite) and Fsp (albite, anorthite, and orthoclase) components.

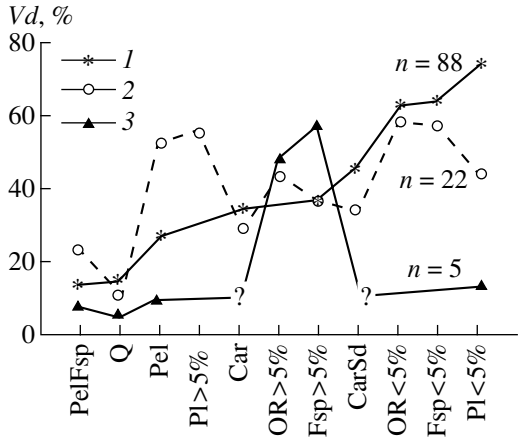

Fig. 7. Discrepancy between modal and normative mineral compositions (*Vd*, rel %). (1) Russian Platform (Ronov *et al.*, 1990, 1995); (2) Siberian Platform (Rosen *et al.*, 1999); (3) Australian Platform (Mumme *et al.*, 1996); (CarSd) sum of calcite, dolomite, ankerite, rhodochrosite, and siderite; (Pl) sum of albite and anorthite. Other symbols are as in Fig. 6.

Center (Potsdam, Germany) (Ronov *et al.*, 1972; 1990). Similar results were obtained for most components in the sample selection of Riphean rocks from the Siberian Platform. The highest *Vd* value of ±53–59 rel % was obtained for feldspars and clay minerals analyzed at the All-Russia Institute of Mineral Resources (VIMS) in Moscow.

Low discrepancy for components calculated at the final allocation stage, when only the residue from preceding calculations is used, serves as an important evidence for the high reliability of normative computation. The good consistence was established for quartz (*Vd* = ±5–15 rel % in all cases) and the sum total of calcite and dolomite. The control CO_2 estimates based on normative minerals are in a satisfactory agreement with results of the bulk chemical analysis (Fig. 6). The highest errors (*Vd* = 60–70 rel %) are related to low (<5 wt %) feldspar contents.

Example of Normative Mineral Calculation and Verification of the Calculated Chlorite Formula

Table 5 shows an example of computation based on the MINLITH algorithm for the mudstone sample studied by Mumme *et al.* (1996). They balanced the chemical composition of the rock and its modal mineral composition, which was estimated with the help of microprobe and XRD methods, by a special petrochemical calculation. The sequence of operations 1–11 and notes in Table 5 demonstrate the details of the MINLITH algorithm work. The accuracy of results is quite satisfactory. The normative and modal illite contents were estimated at 44.05 and 45.3 wt %, respectively. The respective values are 40.58 and 45.1 wt % for quartz, 9.48 and 5.6 wt % for chlorite, and 3.68 and 3.80 wt % for albite. The normative pyrolusite (0.92%), rutile (0.73 wt %), and carbonaceous matter were not found among modal minerals, probably due to an insufficient detection limit of the microprobe or scattering of these components within the prevailing chlorite and illite. The normative serpentine (0.01%) likely indicates a Mg excess in chlorite.

The following formula of chlorite expressed in oxides was obtained from the computer analysis (Table 5): $2.72MgO\ 1.98FeO\ 1.28Al_2O_3\ 2.75SiO_2\ 4H_2O$. The special command converts it into the traditional form $(Mg_{2.72}Fe_{1.28})_4\ (Fe_{0.70}Al_{1.30})_2\ (Al_{1.26}Si_{2.75})_4\ O_{10}\ (OH)_8$, which can directly be compared with its modal counterpart $(Mg_{2.64}Fe^{2+}_{1.36})_4\ (Fe^{3+}_{0.38}Al_{1.58})_2\ (Al_{1.3}Si_{2.7})_4\ O_{10}\ (OH)_8$ (Mumme *et al.*, 1996, Table 2, Sample S3). Both formulas are approximately identical.

The results turn out to be worse if the modal chlorite contains a considerable amount of mixed-layer component and absorbed cations. For the graywacke sample (Mumme *et al.*, 1996, Table 2, Sample S5) with 11.2 wt % of modal chlorite, the normative chlorite was estimated at 13.19 wt %. The comparison of both formulas demonstrates only a rough similarity:

normative $(Mg_{2.08}Fe_{1.92})_4\ (Fe_{0.77}Al_{1.23})_2\ (Al_{1.29}Si_{2.71})\ O_{10}\ (OH)_8$

modal $[K_{0.03}Na_{0.02}Ca_{0.07}]_{0.12}(Mg_{1.6}Mn_{0.01}Fe_{2.36})_{3.97}(Al_{1.17})_{1.17}(Al_{0.88}Si_{3.12})_4\ O_{10}(OH)_8$.

Table 5. Example of MINLITH calculation (normative mineral composition of mudstone vs. modal composition)

Component	Bulk chemical composition, wt %	Sequence of operations and normative minerals[1]										
		1	2	3	4	5	6	7	8	9	10	11
		Molecular quantity	C_{org}	RT	PR	AB	CHL	ILL	OR	SRP	PRL	Q
SiO_2	66.57	11078				416.22	422.79	3453.16	40.705	79.89		6665.21
TiO_2	0.73			–								
Al_2O_3	17.9	1676				69.37	196.99	1402.85	6.78			
Fe_2O_3	0.85											
FeO	3.01											
FeOt	3.78	525			4.055		305.12	215.82				
MnO	0.01	1.41									1.41	
MgO	3.04	754					418.34	215.82		119.84		
CaO	0	0										
Na_2O	0.43	69.37				69.37						
K_2O	4.13	438.4						431.65	6.78			
P_2O_5	0.01	0										
C	0.11		–									
S	0.026	8.11			8.11							
Calculated formula unit					4.055	69.37	154.02	215.82	6.78	39.94	1.41	6665.21
Calculated wt %			0.11	0.73	0.05	3.64	9.36	43.48	0.38	0.01	0.91	40.05
Calculated wt % corrected to 100%			0.11	0.74	0.05	3.68	9.48	44.05	0.38	0.01	0.92	40.58
Modal composition, wt %[2] (after Mumme *et al.*, 1996)						3.8	5.8	45.3				45.1

Notes: [1] Comments to operations:

(1) **Preparation:** calculation of FeO_{tot} and molecular quantities (oxide wt %/molecular weight) × 10000.

(2–4) **Calculation of accessory components.** Conversion of TiO_2 into RT and C_{org} into C; calculation of PR from the calculated formula unit $S^0/2$ and calculation of residue ($Fe^1 = Fe^0–Fe_{PR}$).

(5–8) **Calculation of aluminosilicates.** Calculation of coefficients (F = 0.41 and A = 0.72) and construction of chlorite formula $2.72MgO \cdot 1.98FeO \cdot 1.28Al_2O_3 \cdot 2.75SiO_2 \cdot 4H_2O$. Fitting of mineral assemblage (Table 3, stage 2, gradation 3): AB, OR, ILL, CHL. (5) Calculation of AB from the calculated formula unit (Na^0); alumina content decreases: $Al^1 = Al^0–Al_{AB}$. (6) Solution of the equation system: $Al^1 = Al_{OR} + Al_{ILL} + Al_{CHL}$; $Mg^0 = Mg_{ILL} + Mg_{CHL}$; $K^0 = K_{OR} + K_{ILL}$ (Table 3, stage 3, gradation 3) and determination of the calculated unit of chlorite from the Mg content: $CHL = (K^0 + 4.5Mg^0 – Al^1)/(4.5k1 – k3)$. The test for adequacy of K_2O, Al_2O_3, and FeO for other minerals. Fe deficiency for the subsequent computation has been detected; the calculated formula unit of chlorite is recalculated to Fe: $CHL = (K^0 + 4.5Fe^1–Al^1)/(4.5k2 – k3) = 154.02$; and Mg is in excess. (7) The illite formula unit is calculated from Fe residue: $ILL = Fe_2 – Fe_{CHL} = 215.82$. (8) Orthoclase is determined from K residue: $OR = K^0–K_{ILL} = 6.78$.

(9–11) **Calculation of residual components.** They correspond to group II 2a based on relationships (Table 4). (9) The Mg residue is allocated to serpentine: $SPR = Mg_n/3 = 39.94$. (10) Mn is recalculated to pyrolusite: $PRL = MnO = 1.41$. (11) The Si residue is treated as quartz: $Q = Si_n – Si_{SRP} = 6665.21$.

[2] Minerals shown as ILL: muscovite (41.0), kaolinite (2.4), and phlogopite (1.9). Minerals shown as CHL: chlorite (5.6) and goethite (0.2). The contents are given in wt %.

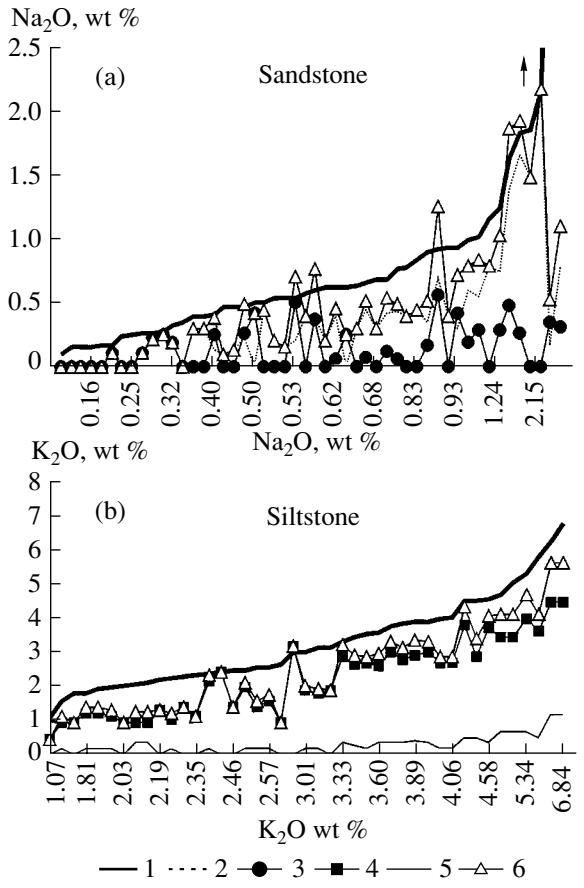

Fig. 8. Discrepancy between (a) Na_2O and (b) K_2O contents based on the bulk chemical composition of rock and calculated from compositions of the respective mineral phases (the amount of phases was determined by the XRD method). (1) Contents based on chemical analysis; calculated Na_2O content (plot *a*) in (2) plagioclase and (3) montmorillonite; calculated K_2O content (plot *b*) in (4) illite and (5) potassium feldspar; (6) total oxide content in minerals. Results of 50 analyses of sandstone (Ronov *et al.*, 1995) and 42 analyses of pelitic rocks (Ronov *et al.*, 1990) are arranged along the x-axis in increasing order (out of scale).

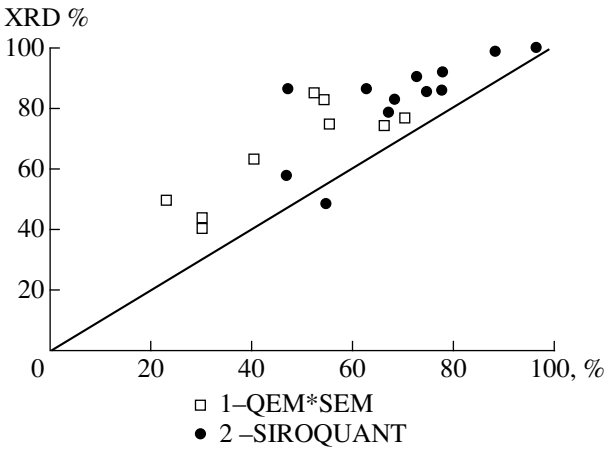

Fig. 9. Discrepancy in kaolinite contents based on different methods. (XRD) X-ray diffractometry; (1) QEM*SEM method (Creelman and Ward, 1996); (2) X-ray diffractometry (Rietveld version) with chemical control by the SIROQUANT method (Ward and Taylor, 1996).

For the time being the statistical correlation of normative and modal chlorite formulas is impossible, because of a scarcity of publications containing both bulk chemical and modal mineral compositions together with chlorite formulas for the same sample. The data presented above allow us to regard the calculated chlorite formulas as a satisfactory approximation.

We should also dwell on correlation of the normative calculation accuracy, which was statistically estimated in the present work, and the precision of the determinations used as reference (standard) modal compositions. Accuracy estimates presented above are quite comparable with the precision of results obtained from the usual XRD method with an uncertainty of 5–20%. This precision was obtained for standards composed of pure minerals and their simple blends. Sedimentary rocks have a more complex composition, and the XRD accuracy hardly attains 5–20% for such rocks. Serious discrepancies are actually revealed during a comparison of the distribution of chemical elements in minerals determined by the XRD method and the bulk chemical composition of the rock. For example, if Na_2O and K_2O are allocated according to the quantities of respective minerals determined by the powder XRD method (Fig. 8), 10–30% of these oxides turn out to be excess quantities, indicating an insufficient accuracy of XRD results. An underestimation of feldspars is also quite possible. The cause of significant errors in feldspar determinations by the MINLITH program probably lies in such underestimation.

Other methods also reveal substantial errors in the powder XRD determinations. Creelman and Ward (1996) applied the QEM*SEM (Quantitative Evaluation of the Mineral matter*Scanning Electron Microscope) technique, an automated BSE scanning system producing a digital image of element concentration on the sample surface. A more accurate information is also provided by the SIROQUANT method that uses XRD results processed with the least square method (Rietveld method) in combination with a petrochemical control with the SEDNORM program (Cohen and Ward, 1991; Ward and Taylor, 1996). The application of both high-precision methods showed that the overestimation reaches 100 rel % for well-crystallized phases (e.g., kaolinite) determined by the XRD method (Fig. 9).

Taking into account the above statements, the relative uncertainty of MINLITH calculations can be accepted as 5–15%. This value increases to 60–70% only for mineral admixtures (<5 wt %). Let us compare these values with results of examination of the reliability of quantitative estimates of mineral compositions in petrology (Hill *et al.*, 1993). The sim-

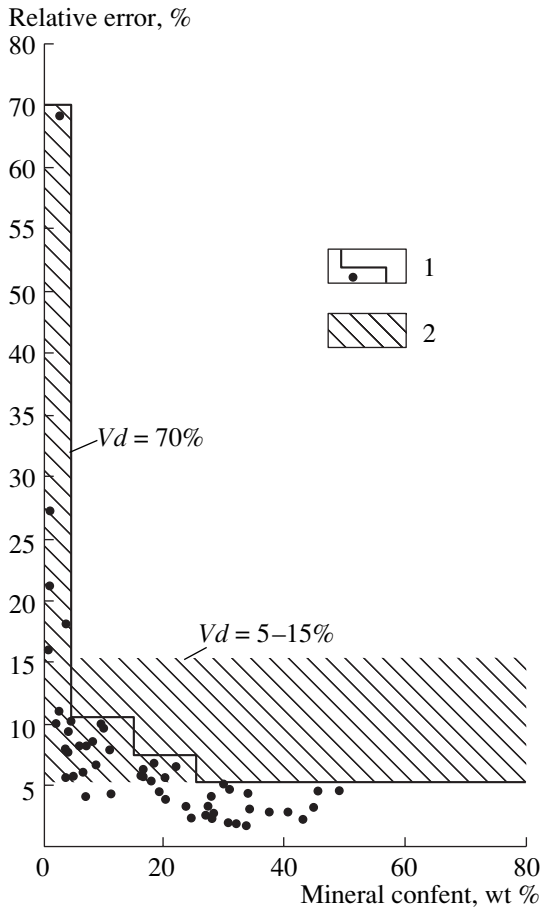

Fig. 10. Relative error (%) vs. mineral content (wt %). (1) Errors estimated as a difference of duplicate measurements using XRD (Rietveld version) and microprobe methods (Hills *et al.*, 1993) coupled with control by the bulk chemical analysis; (2) region of relative errors of MINLITH calculations (*Vd*) deduced from the statistical comparison of mineral norms and modes.

plest mineral compositions of granite and gabbro were checked by duplicate measurements (estimate of reproducibility). Each measurement was based on XRD (Rietveld version) and microprobe analyses along profiles with estimates of the composition of present phases controlled by the bulk chemical analysis (Hill *et al.*, 1993). The reproducibility error was 1–5 rel % for mineral contents of 25–50 wt %, 7 rel % for mineral contents of 15–25 wt %, 10 rel % for mineral contents of 5–15 wt %, and up to 67 rel % for mineral contents of ≤5% wt %. The uncertainty of MINLITH results accepted above is 5–15 rel %, which is comparable (although significantly higher) to that for the high-precision granite and gabbro measurements. The significant errors are similar (60–70 rel %) for minor contents of accessory phases (≤5% wt %). Uncertainties in the quantitative determination of mineral composition are compared in Fig. 10.

CONCLUSIONS

The MINLITH program allows one to calculate the normative mineral composition of sedimentary rocks and their metamorphic counterparts. This universal method can be applied to most types of sedimentary rocks, including clastic, pelitic, and carbonate varieties, based on a limited set of minerals and their simplified compositions. The program comprises a great number of arithmetic operations making up an algorithm. Each operation solves the equations allocating the major oxides to possible (expected) normative minerals. The operation sequence is determined from empirical relationships based on the study of numerous reference samples.

The accuracy of MINLITH calculations was statistically estimated from comparison with results of the high-precision study of modal mineral compositions. In most cases, uncertainty lies within a range of 5–15 rel % and attains 60–70 rel % if the mineral content is below 5 wt %. It is evident that the MINLITH program is a rather simple, convenient, and helpful tool for the approximate estimation of mineral compositions of sedimentary rocks for lithological purposes.

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REFERENCES

Aksamentova, N.V., Some Problems of the Procedure for Processing Analyses of Geochemical Samples, *Voprosy geologii tverdykh poleznykh iskopaemykh* (Problems of the Geology of Solid Mineral Resources), Minsk: Belorus. Nauchno-Issled. Geol.-Razved. Inst., 1975, pp. 145–161.

Aksamentova, N.V., Rosen, O.M., Trusov, A.I., and Abbyasov, A.A., Primary Composition of Rocks in the Iron Ore Sequence of the Okolov Group in the Belorussian Crystalline Basement, *Dokl. Nats. Akad. Nauk Belarusi*, 2002, vol. 45, no. 6, pp. 106–110.

Avidon, V.P., *Koeffitsienty dlya mineralogicheskikh i petrokhimicheskikh pereschetov* (Coefficients for Mineral and Petrochemical Recalculations), Moscow: Nedra, 1976.

Caritat, P., de Bloch, J., and Hutcheon, I., LPNORM: A Linear Programming Normative Analysis Code, *Comput. Geosci.*, 1994, vol. 20, pp. 313–347.

Cohen, D. and Ward, C.R., SEDNORM - A Program to Calculate a Normative Mineralogy for Sedimentary Rocks Based on Chemical Analyses, *Comput. Geosci.*, 1991, vol. 17, pp. 1235–1253.

Creelman, R.A. and Ward, C.R., A Scanning Electron Microscope Method for Automated, Quantitative Analysis of Mineral Matter in Coal, *Int. J. Coal Geol.*, 1996, vol. 30, pp. 249–269.

Currie, K.L., GENORM: A Generalized Norm Calculation, *Comput. Geosci.*, 1991, vol. 17, pp. 77–89.

Hill, R.J., Tsambourakis, G., and Madsen, I.C., Improved Petrological Modal Analyses from X-Ray Powder Diffraction Data by Use of the Rietveld Method. Part I. Selected

Igneous, Volcanic and Metamorphic Rocks, *J. Petrol.*, 1993, vol. 34, pp. 867–900.

Kolka, R.K., Laird, D.A., and Nater, E.A., Comparison of Four Elemental Mass Methods for Clay Mineral Quantification, *Clays Clay Miner.*, 1994, vol. 42, pp. 437–443.

Kossovskaya, A.G. and Shutov, V.D., Problem of Epigenesis, *Epigenez i ego mineral'nye indikatory* (Epigenesis and Its Mineral Indicators), Moscow: Nauka, 1971, pp. 9–34.

Laird, D.A. and Dowdy, R.N., Simultaneous Mineralogical Quantification and Chemical Characterization of Soil Clays, *Clays Clay Miner.*, 1994, vol. 42, pp. 745–754.

Merodio, J.C., Spalletti, L.A., and Bertone, L.M., A FORTRAN Program for the Calculation of Normative Composition of Clay Minerals and Pelitic Rocks, *Comput. Geosci.*, 1992, vol. 18, pp. 47–61.

Mumme, W.G., Tsambourakis, G., Madsen, I.C., and Hill, R.J., Improved Petrological Modal Analyses from X-Ray Powder Diffraction Data by Use of the Rietveld Method. Part II. Selected Sedimentary Rocks, *J. Sed. Res.*, 1996, vol. 66, pp. 132–138.

Nalimov, V.V., *Primenenie matematicheskoi statistiki pri analize veshchestva* (Application of Mathematical Statistics for the Analysis of Material), Moscow: Gos. Izd. Fiz.-Mat. Liter., 1960.

Pactunc, A.D., MODAN: An Interactive Computer Program for Estimating Mineral Quantities Based on Bulk Composition, *Comput. Geosci.*, 1998, vol. 24, pp. 425–431.

Pearson, M.J., Quantitative Clay Mineralogical Analyses from the Bulk Chemistry of Sedimentary Rocks, *Clays Clay Miner.*, 1978, vol. 26, pp. 423–433.

Ronov, A.B., Migdisov, A.A., and Khain, V.E., Reliability of Quantitative Research Methods in Lithology and Geochemistry, *Litol. Polezn. Iskop.*, 1972, no. 1, pp. 3–26.

Ronov, A.B., Migdisov, A.A., and Khane, K., Problem of the Distribution and Mineral Composition of Clays in the Sedimentary Cover of the Russian Platform, *Geokhimiya*, 1990, no. 4, pp. 467–481.

Ronov, A.B., Migdisov, A.A., and Khane, K., Quantitative Regularities of Compositional Evolution of Silty–Sandy Rocks in the Russian Plate, *Geokhimiya*, 1995, no. 3, pp. 323–348.

Rosen, O.M. and Nistratov, Yu.A., Determination of the Mineral Composition of Sedimentary Rocks from Their Chemical Analyses, *Sov. Geol.*, 1984, no. 3, pp. 76–83.

Rosen, O.M., Nistratov, Yu.A., Zlobin, V.L., *et al.*, *Metod vychisleniya mineral'nogo sostava osadochnykh i osadochno-metamorficheskikh porod po ikh khimicheskim analizam: obosnovanie i programma dlya EVM* (Method for the Calculation of Mineral Compositions of Sedimentary and Metasedimentary Rocks Based on Their Chemical Analyses: Substantiation and Program for Electron Computer), Available from VINITI, Moscow, 1982, no. 3768.

Rosen, O.M., Abbyasov, A.A., Migdisov, A.A., and Bredanova, N.V., Mineral Composition of Sedimentary Rocks: Calculation from Petrochemical Data (MINLITH Program), *Izv. Vyssh. Uchebn. Zaved., Geol. Razv.*, 1999, no. 4, pp. 21–35.

Rosen, O.M., Abbyasov, A.A., Migdisov, A.A., and Yaroshevskii, A.A., The MINLITH Program for the Calculation of Mineral Composition of Sedimentary Rocks: Reliability of Results Pertaining to Sediments of Ancient Platforms, *Geokhimiya*, 2000, no. 4, pp. 431–444.

Rosen, O.M., Safronov, V.T., and Abbyasov, A.A., Sedimentary Environments of the Amphibolite-Grade Early Proterozoic Keiva and Kukas Basins (North-East Baltic Shield): Normative Mineral MINLITH Analysis, *Precambrian Sedimentary Environments. Spec. Publ. Int. Assoc. Sediment.*, 2002, vol. 33, pp. 259–274.

Shaw, D.M., *Interpretation geochimique des elements en traces dans les roches cristallines*, Paris: Masson et C^{ie}, 1964.

Shutov, V.D., *Mineral'nye paragenezy grauvkkovykh kompleksov* (Mineral Parageneses of Graywacke Complexes), Moscow: Nauka, 1975.

Ward, C.R. and Taylor, J.C., Quantitative Mineralogical Analysis of Coals from the Callide Basin, Queensland, Australia Using X-Ray Diffractometry and Normative Interpretation, *Int. J. Coal Geol.*, 1996, vol. 30, pp. 211–229.

Zlobin, V.N., Rosen, O.M., and Abbyasov, A.A., Two Meta-Sedimentary Basins in the Early Precambrian Granulites of the Anabar Shield (Polar Siberia): Normative Mineral Compositions Calculated by the MINLITH Program and Basin Facies Interpretations, *Precambrian Sed. Environ. Spec. Publ. Int. Assoc. Sediment.*, 2002, vol. 33, pp. 275–292.