

A Linear Programming Approach to Determine the Normative Composition of Sedimentary Rocks¹

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The analysis of modal and normative composition of sedimentary rocks is widely used for studying their sources and tectonic settings. The normative calculation of the mineral composition of rocks in this study is formulated as a linear programming problem and is solved by means of the simplex method. This enables both simultaneous and successive subtraction of a set of basic minerals from a rock sample represented by its chemical composition $\{SiO_2, \dots, LOI\}$. Such an approach provides a more exact calculation of the contribution of basic minerals in the rock. This mathematical approach is used to study two representative sets of sandstones and fine-grained rocks from a Meso- to Neoproterozoic marginal basin of southeastern Siberia (Uchur–Maya region, Yakutia) and a Pennsylvanian-Lower Permian uplifted continental block in Colorado, USA. The calculated normative mineral compositions of the Siberian sandstones are consistent with the observed modal compositions. These sandstones vary from K- Feldspar rich arkoses at the base of the sequence (the Uchur Group, lower Riphean) to quartz arenites or lithic sandstones and wacke in transgressive successions of the middle-upper Riphean. Arkoses and quartz arenites are dominant in Meso- to Neoproterozoic Siberia. These samples represent craton interior uplifted basement and quartzose, recycled orogen provenance of a stable craton in Rodinia. There are higher but consistent discrepancies between the calculated and observed compositions for the Pennsylvanian to Lower-Permian arkoses and quartz arenites (Sangre de Cristo, Belden, and Maroon Formations). The differences between the predicted and observed mineralogy may be due to uncertainties in the modes in the matrix and cement of the sandstones. This normative program should supplement modal calculations and provide better genetic constructions, especially in case of matrix-rich sandstones.

KEY WORDS: chemical analysis, normative calculation, linear programming, sedimentary rocks.

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INTRODUCTION

The study of the primary mineral composition of sedimentary rocks is important to understand the evolution of sources and environments of coarse-grained clastic sequences (Condie, 1993; Dickinson, 1985; Dickinson and Suczek, 1979; Ingersoll and others, 1984). The mineralogy of shales and siltstones reflects weathering conditions and diagenesis and does not necessarily represent that of the source (Cox and others, 1995; Cox and Lowe, 1996; Cullers, 1995, 2000; Cullers and Podkovyrov, 2000). The chemical composition of shales and siltstones may be used for source reconstructions (Nesbitt and others, 1996), but it requires evidence from independent quantitative models including normative mineral composition calculations especially in the case of more altered sediments.

The quantitative reconstruction of the primary minerals of sediments in sedimentary rocks may be estimated by the classic modes of thin sections or by joint X-ray studies and microprobe analysis of the minerals. The normative mineral decomposition of sedimentary rocks is based on chemical analyses of rocks, and the normative calculations require more or less reliable assumption about (1) the constituent minerals especially in the case of matrix- or clay-rich samples with advanced diagenetic transformations and (2) a predetermined order of their subtraction, i.e. about degree of importance of those minerals for a given rock type (Cohen and Ward, 1991; Cox and Lowe, 1996).

The purpose of this study is to develop the algorithm for the normative decomposition proceeding from the most general approach to this problem as a petrological mixing one. There are some studies devoted to special cases of the same problem (see, e.g., Cox and Lowe, 1996, (p.558, Appendix); Rosen, Abbysov, Migdisov, and Yaroshevsky, 2000; Rosen and Nistratov, 1984). In works of such kind a calculation scheme of the normative analysis is suggested for some particular cases (for instance a special type of rock). And according to this scheme the supposed constituent minerals are subtracted each in turn from a rock sample. Intended for a concrete case this scheme gives a good agreement of normative and observed modal compositions. But when the order of mineral subtractions is not obvious this approach does not allow to estimate the simultaneous contribution of "competing" mineral phases (the phases including identical components such as K_2O in potassic feldspar and hydromica (illite)). The proposed approach to the decomposition do not suffer from this disadvantage.

METHOD

The mixing problem can be considered as a topic of linear programming. For formulation of the mathematical model of the problem, let us suppose that a sample of a rock is represented by a sequence of the mass contents of r oxides:

(m_1, m_2, \dots, m_r) . Also, each mineral from a fixed set (basis) of s minerals, which are assumed to enter into the rock, is represented by the same rock-forming oxides. We shall characterize j th mineral ($j = 1, 2, \dots, s$) by a sequence of numbers $(t_{1j}, t_{2j}, \dots, t_{rj})$ where t_{ij} is the molecular weight of the i th oxide in that mineral. If x_j is the number of moles of the j th mineral included in a sample then obviously the following system of inequalities take place:

$$t_{i1}x_1 + t_{i2}x_2 + \dots + t_{is}x_s \leq m_i, \quad i = 1, 2, \dots, r \tag{1}$$

A solution of this system (x_1, x_2, \dots, x_s) should naturally satisfy the condition of nonnegativity $x_j \geq 0$ for $j = 1, 2, \dots, s$. The system of inequalities (1) has an infinite number of solutions and it is necessary to enter some criterion of optimality for choice among these solutions. Let us enter additional variables y_1, y_2, \dots, y_r such that the inequalities (1) will be transformed to system of the following linear equations:

$$t_{i1}x_1 + t_{i2}x_2 + \dots + t_{is}x_s + y_i = m_i, \quad i = 1, 2, \dots, r \tag{2}$$

Thus all $y_i \geq 0$ and in our case y_i means the residual of the i th oxide after subtracting the basic minerals in quantity x_1, x_2, \dots, x_s moles from the rock. Now the task can be formulated to find such solution $(x_1, x_2, \dots, x_s, y_1, \dots, y_r)$ of the system (2) which is subject to the constraints $x_j \geq 0, y_i \geq 0$ ($j = 1, 2, \dots, s; i = 1, 2, \dots, r$) and minimizes the sum $\sum_{i=1}^r y_i$. And it is a problem of linear programming. Such a problem has been investigated thoroughly and there are algorithms for its solution (for example, see Josephson, 1964).

The system (2) can be transformed to a dimensionless form. For this purpose the coefficients at x_j in each equation of the systems (2) are divided by the sum $f_j = t_{1j} + t_{2j} + \dots + t_{rj} + l_j$ and so on for all j ($j = 1, 2, \dots, s$) where the quantity l_j is a total molecular weight of H_2O and other volatile components included in the formula of the j th mineral. Thus the quantity f_j represents a molecular (formula) weight of the j th mineral. Now the unknown variables should be considered as taking new form namely $x'_j = f_j x_j$ ($j = 1, 2, \dots, s$). These variables represent mass contents of the appropriate minerals in a sample. Dividing both sides of Eq. (2) by the sum of all m_i transforms the right side of the system (2) to relative weight values $b_i = m_i / \sum m_j$. Evidently the collection of quantities b_i ($i = 1, 2, \dots, r$) is a customary bulk chemical analysis. Let the new coefficients of the system be $a_{ij} = t_{ij} / f_j$ and the unknowns x_i, y_i signify the quantities $x'_i / \sum m_j$ and $y_i / \sum m_j$. Then finally the problem is formulated to find the solution of the system of the equations

$$a_{i1}x_1 + a_{i2}x_2 + \dots + a_{is}x_s + y_i = b_i, \quad i = 1, 2, \dots, r \tag{3}$$

such that all x_i and y_i are nonnegative and the value $\sum_{i=1}^r y_i$ is minimized. Of course this choice of an object function is arbitrary to some extent but it seems to be most natural. Other object functions are mentioned below.

Such a formulation of the problem provides both a successive (as in Rosen and others, 1984, 2000) and parallel (simultaneous) process of subtraction of the normative minerals from the chemical analysis of rock. In the first case some priority among minerals of the basis should be established depending for example on the type of rock. The minerals having a higher priority are subtracted first. For subtracting the next minerals the same problem is solved with a new set of coefficients a_{ij} calculated for these minerals and new right-hand side of system (3). The remains of sample oxides after the previous stage (i.e., part (y_1, \dots, y_r) of the previous solution) are the right-hand side of the new system. The parallel process means simultaneous subtraction of several minerals of equal priority. In this case if some minerals have in their formula identical oxides, the algorithm of the solution provides an optimum distribution of these oxides between "competing" minerals in the sense of a minimum of the sum of the residuals of oxides. Certainly it is possible to combine these both processes, in other words at some stages of a successive process to subtract several minerals simultaneously.

It is necessary to remark that the volatile components (H_2O , CO_2 , etc.) included in chemical formulas of some minerals of the basis may produce some inaccuracy in the final result. They may insert some inaccuracy in the end result. For correct consideration of the problem it would be necessary to add to the system of inequalities (1) similar inequalities for volatiles and to solve the problem taking into consideration the extended system. But it is not possible because in the usual chemical analyses the volatile components enter as a total value of LOI. Therefore there is nothing but to assume that for any solution of the problem (2) these "not added" inequalities would be satisfied, or in other words that volatile components in a rock sample are in abundance.

This remark seems to be important because consideration of these oxides in the formulas of minerals (value l_j in the formula for f_j) and actually ignoring them in the analysis can result in a breach of normalization of the solution, i.e. the sum of components of the solution will differ from a unit. It is easy to show that this will not happen if just the "solid" part of the mineral formula is considered (for f_j proposed $l_j=0$) and a chemical analysis renormalized to a unit. Or else, because only relative values of the contents of basic minerals in rock are of interest, the final solution must be normalized.

Attempts to consider the problem of decomposition over mineral basis as an optimization problem within the scheme of the linear model (a vector sample is represented as a linear combination of vectors describing minerals from a basis) had been undertaken before (Leontyev and Karpov, 1975; Predovsky and Martynov, 1980; Wright and Doherty, 1970). Some measure of approximation of a vector

(the chemical analysis of rock) by a linear combination of predefined vectors (a mixture of the basic minerals) is characteristic for this class of problems and its value depends on the difference between these vectors.

As such measure Leontyev and Karpov (1975) used the maximal value of component misfit of the above vectors. Minimization of the sum of squares of all component misfits (the least squares method) is used in Predovsky and Martynov (1980). Besides the computational difficulties which happen with these both approaches to the problem another shortcoming can be pointed out—these models permit negative solutions. In the context of the problem the negative proportions of mineral phases have no reality.

The models considered by Wright and Doherty (1970) and Banks (1979) do not possess this disadvantage. In both works, the authors impose a constraint of nonnegativity upon that part of possible solution which relates to mineral content, i.e. (x_1, \dots, x_s) , but the residuals (y_1, \dots, y_r) are allowed to be of either sign. And the latter is the most important distinction between the present approach and theirs⁵.

If it could be assumed that a considered rock in itself is a mixture of a definite set of minerals and only computational errors lead to discrepancy between the rock and some linear combination of these minerals then the both models can be employed (the fitting problem). Moreover it is not very important which object function is used namely L_2 —the sum of the squares of the residuals (Wright and Doherty, 1970) or L_1 —the sum of the absolute values of the same residuals (Banks, 1979). Really these functions are tightly connected with each other by the relations $(1/\sqrt{r})L_1 \leq \sqrt{L_2} \leq L_1$ and it can be seen that minimization one of them results in minimization another. In practice the upper assumption is rather uncertain. In the case of a real rock it seems more realistic to get a notion about the principal minerals forming this rock type than about the whole mineral composition. In our approach, if after subtraction of a mixture of these principal minerals by any optimal method there remain some components (oxides) of the chemical analysis then we can try to construct another mixture of some minor minerals. It seems that the question about a “hierarchy” of minerals in some set cannot be passed over by examining a sufficiently numerous basic minerals and assembling them for some rock type. A priori equivalence attributed to basic minerals may result in distortions of the true geological situation.

Thus, the first and essential stage in the problem of decomposition of the chemical analysis of a rock sample over a normative basis should be to establish a priority order in the set of normative minerals. In other words it is necessary to point out the greater or lesser importance of a normative mineral for some

⁵The statistical speculations by Banks (1979) are of no account because the origins of them are not proved for the subject of research. For instance the normal distribution that is a basis of his statistical estimations takes place when components of a rock sample are independent. But it is doubtful to be assumed for a real sample.

type of rock. An example of such ordering for sedimentary rocks is given in Rosen and Nistratov (1984). We use just this ordering in the further normative calculations.

THE DATA AND GEOLOGICAL BACKGROUND

For the analysis of the method, two sets of sedimentary rocks have been analyzed for modal minerals in thin sections and for major element oxides. The major elements were analyzed by atomic absorption (Shapiro and others, 1978) and X-ray fluorescence with precision of most oxides better than $\pm 5\text{--}8\%$. The mineralogy of the silt and sand fractions were determined by counting about 500 points in immersion oils, partly stained for potassium feldspar (Cullers, Colorado samples) or by counting in thin sections on the Andin integrated table (transect of 500–600 grains, Podkovyrov, Uchur–Maya samples). For comparison, some samples of sandstones and shales have been analyzed for mineral compositions by X-ray and microprobe methods. The first example are of the Riphean–Vendian (Meso and Neoproterozoic) sandstones from the southeastern Siberian craton sequences in Russia. This Late Proterozoic cover sequence (3.5 to 15 km thick) from the Uchur–Maya region of the southeastern Siberian platform spans a time interval of about 1000 Ma (< 1600 to 542 Ma). This sequence contains mostly shallow to open shelf, epicratonic terrigenous and carbonate deposits with various compositions of sandstones and shales (Cullers and Podkovyrov, 2000; Kotova and Podkovyrov, 2001; Semikhatov and Serebrykov, 1983). Arkoses and quartz arenites dominate in these successions as a part of the Rodinia landmass. They represent interior, uplifted basement and quartzose, recycled orogen provenance of a stable craton.

The degree of secondary transformations of the Uchur–Maya deposits varies from moderate diagenetic alterations of Maya River rocks in the western portion ($2M_1$ and $1Md$ illite, chlorite with mixed layer illite-smectite, kaolinite, pyrophyllite, calcite, and hematite association in shales) to a deeper burial in the Yudoma–Maya depression shales to the east. The eastern deposits contain muscovite-type mica, with minor chlorite, quartz, pyrophyllite, and hematite (Cullers and Podkovyrov, 2000).

The Uchur–Maya samples represent predominate types of sandstones in the sequence. The sandstones consist mostly of monocrystalline quartz and feldspar with minor rock fragments (including polycrystalline and slaty quartz aggregates), muscovite (or illite to muscovite phases), opaque minerals and 15–55% of matrix, and cement composed mainly of illite, chlorite quartz, and carbonate (Tables 1, 2). The modes in standard QFL diagrams (Dickinson and Suczeck, 1979) plot in the transitional to interior craton region. The sandstones range from K-feldspar rich in Lower Riphean successions (samples 54-32 to 59-17) to more plagioclase rich in the less mature lithic arenites of the Middle Riphean Totta Formation (samples

55-73 to 56-13). Sample 74-9 is from the weathering crust of the uppermost Totta sequence, and it is a diagenetically altered, carbonaceous quartz arenite. The Upper Riphean Ui Group samples are matrix rich, mostly plagioclase wackes (samples 85-3, 85-20) with abundant chlorite in the matrix. These samples are arkosic (10–16% Or, 17–22% Pl, samples 86-5, 86-9, 104-43) and subarkosic to quartz, partly carbonaceous arenites (samples 71-1, 71-12, 104-40, 104-47, Table 2).

The samples with the highest clastic potassic feldspar and lowest plagioclase in the Lower Riphean sandstones have X-ray data for samples 54-32 (40–45% Or, <5% Pl) and 57-13 (30–40% Or, traces of Pl) that is in good agreement with the norm calculations (Table 3). Moderate, but systematic discrepancies between petrographically observed (Table 2) and calculated (Table 3) amount of K-mica (illite) usually reflect higher K₂O content in the 2M₁ illite- to muscovite micas (8.5–11.2% accordingly to microprobe data, samples 54-32, 59-17, 85-20) than the 6.6–7% in the accepted illite formula. The appearance of serpentine in calculated compositions (Table 3, 0–9.52%) correlates to detected amounts using X-ray data only for samples 57-13, 57-57, and 59-17. Samples with a high amount of observed chlorite in the matrix (30% in 85-3 and 33% in 85-20, Table 2) have normative amounts of chlorite that are close to the observed amount of chlorite (28% and 38.5%, Table 3). This suggests that these are good norm values for chlorite-rich samples despite presence of some normative quantities of serpentine that is an agreement with microprobe data (more high-Mg chlorite in samples compare with chlorite composition in the base).

Concentrations of opaque minerals observed in the samples (Table 2) are in good agreement with calculated goethite norms (Table 3). Several samples analyzed by X-ray data have good agreement between norms and modes (e.g., 5–7% magnetite and hematite in sample 74-29 comparably with 7% modal ore minerals). Discrepancies may be observed between calculated norm and modal amounts of glauconite because of lack of glauconite composition in the basis (X-ray data of samples 56-13 and 104-43 suggest that they may contain <5% glauconite each).

The second example includes sandstones of Pennsylvanian-Permian age, Colorado, USA. A series of shales and sandstones found near the source from the central Colorado (the Belden, Sangre de Cristo, and Maroon Formations) were examined petrographically and were analyzed for major and selected trace elements (Cullers, 2000) (Table 4, 5). Sediments of these formations were derived from adjacent uplifts of mostly granitoid basement, and were deposited in the north-south trending Colorado trough (De Voto, 1980; Lindsey, Clark, and Soulliere, 1987). The Belden Formation consists mostly of dark shale was deposited in shallow marine or deltaic environment and also contains minor feldspathic sandstones and limestones (De Voto, 1980; Johnson, 1987). The Maroon and Sangre de Cristo sequences up to 2000–4600 m in thickness consist of arkosic sandstones, conglomerates, siltstones, and shales, deposited in arid conditions in

Table 1. Chemical Composition of the of the Riphean–Vendian sandstones, Uchur–Maya Region, Southeast Siberia ($n = 21$)

Sample number	SiO ₂	TiO ₂	Al ₂ O ₃	SFeO	MnO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅	LOI	Total
54-32	79.08	0.33	9.09	1.82	0.04	0.10	0.58	0.90	6.55	0.13	0.85	99.47
54-45	60.84	0.10	4.79	0.96	0.01	6.20	8.61	0.61	3.30	0.02	14.04	99.48
57-13	65.85	0.50	13.48	4.92	0.01	3.54	0.28	0.15	7.98	0.02	2.77	99.50
57-15	63.90	0.79	16.26	3.10	0.01	3.48	0.16	0.10	8.79	0.09	2.83	99.51
58-11	77.18	0.20	10.61	2.31	0.01	1.41	0.20	1.13	5.16	0.10	1.20	99.51
58-15	70.40	0.21	8.48	3.54	0.03	2.68	4.18	1.00	3.48	0.05	5.45	99.50
58-16	72.96	0.30	10.53	3.20	0.01	1.80	2.05	1.70	4.08	0.14	2.72	99.49
59-17	59.89	0.25	9.70	3.26	0.01	8.08	5.04	0.11	5.39	0.10	7.67	99.50
55-73	79.78	0.25	8.21	5.10	0.02	0.85	0.35	1.59	1.77	0.12	1.39	99.43
74-29	71.79	0.76	11.77	6.47	0.01	1.34	0.46	2.30	2.09	0.09	2.41	99.49
56-13	76.97	0.55	10.37	3.34	0.03	1.02	1.17	2.29	1.83	0.08	1.85	99.50
74-9	67.56	0.01	1.64	4.39	0.40	0.86	12.89	0.01	0.05	0.02	11.71	99.54
71-12	56.05	0.12	6.18	1.84	0.08	2.97	14.24	1.38	2.18	0.06	14.39	99.49
71-1	67.82	0.23	8.03	3.01	0.08	3.16	4.94	1.50	2.69	0.05	7.99	99.50
85-3	72.28	1.27	9.83	5.76	0.17	1.92	2.16	2.39	1.16	0.08	2.00	99.02
85-25	62.46	0.90	16.76	5.86	0.11	3.12	1.26	3.20	2.73	0.16	3.12	99.68
86-5	81.09	0.40	8.72	1.48	0.02	1.21	0.38	2.29	2.68	0.19	1.04	99.51
86-9	72.35	0.31	10.26	1.67	0.02	2.26	3.03	2.16	3.93	0.18	3.34	99.51
104-40	90.22	0.40	4.74	1.01	0.01	0.81	0.24	0.20	1.32	0.26	1.16	100.37
104-43	66.06	0.75	14.90	5.23	0.03	1.92	0.71	2.84	3.84	0.36	3.34	99.99
104-47	71.71	1.02	12.62	4.90	0.05	1.18	0.18	2.00	2.98	0.08	2.00	98.72

Table 2. Modal Composition of the Riphean–Vendian Sandstones, Uchur–Maya Region, Southeast Siberia

Sample number	Q	F		L _t	Total QFL grains (%)	Total matrix and cement	Matrix and cement composition				
		Or	Pl				Ill	Chl	Carb	Opaq.	Qu
54-32	44	31	6	4	85	15	3	0	0	2	10
54-45	31	15	6	4	56	44	0	0	30	1	14
57-13	27	38	4	3	72	28	14	1	0	5	8
57-15	25	32	2	5	64	36	24	3	0	2	7
58-11	40	24	8	5	77	23	10	0	0	2	11
58-15	46	10	9	3	68	32	9	4	10	3	6
58-16	25	15	15	5	60	40	9	0	5	4	22
59-17	8	20	15	2	45	55	18	3	18	4	11
55-73	50	2	15	6	73	27	12	0	0	5	10
74-29	30	0	17	5	52	48	18	2	0	7	11
56-13	42	0	16	7	65	35	14	0	3	3	15
74-9	62	0	0	6	68	34	0	0	26	0	8
71-12	32	8	10	5	55	45	4	0	35	1	5
71-1	43	5	11	6	65	35	11	1	15	2	6
85-3	29	4	15	9	57	43	2	30	2	1	8
85-25	17	3	20	10	50	50	11	33	1	0	5
86-5	48	10	17	5	80	20	6	3	0	3	8
86-9	33	16	20	6	75	25	9	0	9	2	5
104-40	72	0	1	8	81	19	15	1	0	1	4
104-43	23	10	22	8	63	37	20	2	0	4	11
104-47	45	1	15	4	65	35	25	0	0	4	6

Note. Q – total quartz, including polycrystalline; F – total feldspars; L_t – total lithic fragments, excluding polycrystalline quartz; Or – orthoclase, Pl – plagioclase; Ill – total white mica as Illite; Chl – chlorite; Carb – carbonate; Opaq – opaque minerals; Qu – quartz.

alluvial to near-shore environments (De Voto, 1980; Johnson, 1987; Lindsey, Clark, and Soulliere, 1987).

Mineralogy has been determined on representative fine to coarse sandstones. The modes in QFL diagrams (Dickinson and Suczeck, 1979) plot in the transitional to interior craton region (Cullers, 2000). The sandstones of the Belden Formation have a higher quartz content and quartz/total feldspar ration than do those of the Sangre de Cristo and Maroon formations (Table 5). This suggests that detritus in the Belden, including minor clastic micas and chlorite, was weathered enough to have removed more of the feldspar from the original granitoid source than the other two formations or was derived from recycled source. The Sangre de Cristo and Maroon formations contain mostly arkosic sandstones with hematitic clay and clay matrix and occasionally carbonate cement with little or no lithic fragments (Table 5). Its quartz to total feldspar ratio are similar to those of granitoids or granite gneisses, suggesting minimal weathering of these units (Cullers, 2000).

Table 3. Calculated Mineral Compositions of the Uchur–Maya Sandstones

	ab	an	or	ill	chl	rt	ap	dol	ank	srp	gt	cal	qu
54-32	7.66	0.81	38.40	0.99	0.00	0.33	0.31	0.37	0.53	0.00	2.00	0.00	48.60
54-45	5.22	0.55	19.67	0.06	0.00	0.10	0.05	28.13	0.00	0.25	1.20	0.00	44.78
57-13	1.27	0.13	36.18	20.00	0.00	0.50	0.05	0.75	0.00	6.83	5.21	0.00	29.08
57-15	0.85	0.09	36.29	28.94	0.00	0.80	0.21	0.08	0.00	6.66	2.58	0.00	23.49
58-11	9.59	0.35	23.19	13.39	0.00	0.20	0.24	0.00	0.00	2.63	2.27	0.00	48.14
58-15	8.35	0.89	13.74	11.88	0.00	0.21	0.12	11.00	2.06	0.00	2.95	0.00	48.81
58-16	14.31	1.52	17.33	12.05	0.00	0.30	0.33	5.10	0.00	0.99	3.40	0.00	44.68
59-17	0.91	0.10	22.53	15.69	0.00	0.24	0.23	15.73	0.00	9.52	3.25	0.00	31.78
55-73	13.46	0.96	2.39	14.62	0.00	0.25	0.28	0.00	0.00	1.28	5.66	0.00	61.09
74-29	19.53	1.71	0.00	22.43	0.00	0.76	0.21	0.00	0.00	2.05	7.03	0.00	46.28
56-13	19.36	2.05	1.43	16.97	0.00	0.55	0.19	2.14	0.00	0.48	3.37	0.00	53.46
74-9	0.08	0.01	0.30	0.00	6.53	0.01	0.05	1.76	6.50	0.00	0.00	18.99	65.77
71-12	11.64	1.24	10.19	4.80	0.00	0.12	0.14	13.09	5.00	0.00	0.00	15.33	38.45
71-1	12.75	1.35	10.71	9.52	0.00	0.23	0.12	13.63	1.83	0.00	2.57	0.00	47.30
85-3	17.48	1.85	5.42	0.91	27.98	1.10	0.16	0.00	0.97	0.00	0.00	2.05	42.06
85-25	20.40	2.16	4.58	13.70	38.50	0.68	0.29	0.00	0.02	0.00	0.00	0.63	19.04
86-5	19.49	0.66	11.51	8.00	0.00	0.40	0.45	0.00	0.00	2.42	1.49	0.00	55.57
86-9	18.15	1.93	18.86	7.60	0.00	0.31	0.42	7.84	0.00	0.86	1.71	0.00	42.32
104-40	1.69	0.00	0.56	13.09	0.00	0.40	0.44	0.00	0.00	1.26	0.67	0.00	81.89
104-43	24.23	1.20	9.10	24.94	0.00	0.76	0.86	0.00	0.00	3.29	5.41	0.00	30.21
104-47	17.10	0.38	3.16	26.47	0.00	1.03	0.19	0.00	0.00	1.52	4.95	0.00	45.19

Note. Minerals: ab – albite, an – anorthite, or – orthoclase, ill – illite, chl – chlorite, rt – rutile, ap – apatite, dol – dolomite, ank – ankerite, srp – serpentine, gt – goethite, cal – calcite, qu – quartz, kln – kaolinite, mnt – montmorillonite, sd – siderite and mgs – magnesite from the base are absent in calculated norms.

Table 4. Chemical Composition of the Pennsylvanian Sandstones (Cullers, 2000)

Sample number	SiO ₂	TiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MnO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅	LOI
SDC-1	45.4	0.77	13.1	5.64	0.15	5.53	11.45	1.06	3.47	0	13.76
SDC-2	50.6	0.72	14.6	5.61	0.12	4.92	6.72	1.16	4.90	0	10.52
SDC-3	36.0	0.51	8.72	5.29	0.35	5.31	20.62	0.89	2.37	0	19.73
SDC-4	60.7	0.60	13.5	2.66	0.17	2.40	6.49	2.87	4.44	0	6.69
SDC-5	67.0	0.41	13.5	3.74	0.047	2.24	2.14	3.13	4.69	0	3.06
SDC-6	65.2	0.71	14.8	5.34	0.027	3.03	0.87	3.22	4.95	0	2.50
SDC-7	59.5	0.95	16.6	6.57	0.036	4.14	0.80	2.79	5.65	0	3.13
SDC-8	60.3	0.92	17.3	6.03	0.030	3.96	0.73	2.39	5.65	0	3.37
SDC-9	55.1	0.90	14.4	5.59	0.10	3.77	5.96	2.37	4.79	0	7.45
SDC-10	49.1	0.70	12.4	6.59	0.19	3.44	10.36	2.28	3.87	0	10.71
SDC-11	55.4	0.77	13.0	5.42	0.11	3.69	7.20	2.43	4.08	0	8.38
SDC-12	53.7	0.81	13.1	5.31	0.15	2.41	8.69	2.99	4.19	0	8.25
SDC-13	51.6	0.55	10.8	3.12	0.24	1.76	13.22	2.65	3.62	0	12.27
SDC-18	53.7	0.59	6.4	2.01	0.32	2.14	15.94	0.10	2.43	0	5.54
SDC-19	62.4	0.64	12.9	2.83	0.094	2.55	5.39	3.23	3.12	0	5.97
SDC-20	50.1	0.78	12.1	4.56	0.096	5.05	9.16	1.06	3.96	0	12.46
SDC-21	63.1	0.45	13.5	3.17	0.076	1.58	4.56	3.69	4.09	0	4.90
SDC-22	57.8	0.83	12.3	4.28	0.33	2.44	7.31	3.24	2.78	0	8.08
SDC-23	55.5	0.65	10.3	5.09	0.17	2.40	10.32	0.93	2.81	0	11.14
SDC-24	62.0	0.89	14.0	5.32	0.12	3.28	3.44	2.18	3.65	0	5.46
SDC-25	72.9	0.65	12.0	4.77	0.061	0.94	0.38	3.49	3.67	0	1.04
SDC-26	60.6	0.76	11.7	4.86	0.084	4.59	3.69	1.97	4.09	0	7.19
SDC-27	53.0	0.82	15.7	7.32	0.12	4.53	3.16	1.54	6.43	0	7.51
SDC-28	57.6	0.81	13.2	5.37	0.19	3.85	4.19	2.62	4.75	0	7.28
BS-2B	48.8	1.00	19.5	10.32	0.02	6.05	1.00	0.47	3.04	0	9.83
BS-2A	55.2	0.86	19.3	6.73	0.032	4.12	1.92	0.51	4.28	0	6.95
BS-1B	68.5	0.43	7.9	4.01	0.040	2.33	7.10	2.32	0.17	0	7.59
BS-1A	58.6	1.07	17.6	4.53	0.013	2.61	2.07	0.52	2.56	0	10.61
BS-3B	65.6	0.75	14.7	8.52	0.017	2.84	0.52	3.22	0.38	0	3.41
BS-3A	46.9	1.13	21.7	5.72	0.029	3.62	5.02	0.81	3.93	0	11.47
BS-10A	65.1	0.49	10.3	2.78	0.024	5.28	4.00	0.74	3.62	0	7.97
BS-10B	51.7	0.27	5.9	1.49	0.060	5.94	13.82	0.97	3.16	0	16.81
BS-15	24.9	0.41	9.5	2.80	0.063	12.67	19.22	0.27	0.74	0	29.51
BS-16A	91.0	0.17	3.8	2.63	0.067	0.15	0.10	0.03	0.87	0	1.50
BS-16B	31.6	0.59	13.1	4.69	0.086	9.08	13.90	0.12	3.63	0	22.49
M1A	61.1	0.63	12.5	3.14	0.10	0.77	8.34	4.37	2.00	0	6.96
M1B	60.4	0.62	12.7	4.21	0.12	1.36	7.02	3.87	2.49	0	6.84
M2A	65.8	0.63	10.2	3.71	0.052	1.87	6.94	1.64	1.95	0	7.68
M2B	69.5	0.69	10.2	3.37	0.068	1.37	5.24	1.83	2.03	0	6.15
M2D	60.8	0.36	13.8	2.72	0.11	1.20	5.55	2.32	4.03	0	8.25
M3	69.1	0.68	10.8	2.99	0.098	1.34	4.82	2.68	2.93	0	5.15

Note. 0 – not analyzed.

Table 5. The Petrography of Selected Sandra de Cristo, Belden, and Maroon Fms Sandstones, Colorado, USA^a

Sample number	Quartz	Plagioclase	Alkali feldspar	Rock fragm.	Total QFL	Total matrix and cement	Hematitic clay	Mikas and chlorite	Carbonate	Opauques	Quartz
SDC-4	28.8	16.5	42.7	0	88.0	10.4	0	1.2	9.2	0.4	0.4
SDC-5	26.1	26.1	28.9	0	81.1	16.4	5	0.3	9.8	2.2	0
SDC-6	28.9	28.9	30.5	0	88.3	9.3	3.2	1.6	4	0.8	1.7
SDC-7	28.2	27.3	28.7	0	84.2	13.4	13.4	2.4	tr	tr	tr
SDC-8	22.3	19.4	34.7	0	76.4	22.4	20	0.6	0	0.6	0
SDC-12	24.8	19.8	25.7	0	70.3	29.2	17.8	tr	5.5	0.5	tr
SDC-13	22.2	23.3	11.9	0	57.4	42	31.8	0	10.2	0.6	0
SDC-18	33.8	16.2	16.9	0	66.9	32.4	0.6	0.7	31.1	tr	0.7
SDC-19	26.7	25.9	26.8	0	79.4	18.4	0.4	1.3	12.6	0.9	3.6
SDC-21	26.2	31.0	31.9	0	89.1	10.9	1.4	tr	6.1	tr	2.9
SDC-22	20.7	20.2	17.5	0	58.4	41.6	17.5	tr	22.0	0	2.1
SDC-24	21.3	21.8	12.9	0	56.0	43.4	33.5	0.6	6.5	0	2.8
SDC-25	34.9	26.2	34.5	0	95.6	2.7	0.4	0.4	0	1.3	1.9
SDC-26	27.4	26.6	24.9	0	78.9	19.9	11.6	1.2	5.0	0	3.3
SDC-28	17.6	17.6	23.6	0	58.8	38.2	23	3	11.5	0	1.8
BS-1B	44.9	18.2	1	0	64.1	30.4	3.5	3.5	10.2	2	2
BS-3B	32.8	31.9	0.4	0	65.1	23.4	2.2	11.5	0	0	4.4
BS-10E	32.0	7.1	24.9	0.4	64.4	32.4	0	1.2	28.8	0	3.6
BS-16A	71.4	4	0	0	75.4	24.6	4.7	0	0	0	8.6
M1A	24	32.7	20.4	0	77.1	18.8	3.1	1.5	8.2	2.6	3.4
M2D	19.2	18.9	12.1	0	50.2	24.4	3.9	24.4	11.9	tr	1.8
M3	36.5	29.8	23.2	0	89.5	10.5	2.2	0	5.5	tr	1.7

^aModified from Cullers (2000).

Table 6. Normative Composition of the Pennsylvanian Sandstones (n = 41)

Sample number	#	ab	an	or	ill	klh	mmt	chl	rt	ap	dol	ank	srp	gt	sd	mgs	cal	qu
SDC-1	(2)	8.56	0.91	2.78	30.40	0.00	0.00	0.00	0.74	0.00	21.34	12.92	0.00	0.00	0.00	0.00	1.60	20.76
SDC-2	(2)	9.65	1.02	11.76	30.25	0.00	0.00	0.00	0.71	0.00	19.34	1.98	0.00	4.67	0.00	0.00	0.00	20.63
SDC-3	(2)	7.19	0.76	3.18	18.43	0.00	0.00	0.00	0.49	0.00	21.47	13.20	0.00	0.00	0.00	0.00	17.06	18.23
SDC-4	(2)	23.67	2.51	18.41	12.96	0.00	0.00	0.00	0.58	0.00	9.50	6.40	0.00	0.00	0.00	0.00	2.26	23.70
SDC-5	(2)	26.27	2.79	22.09	9.78	0.00	0.00	0.00	0.41	0.00	5.13	0.00	2.07	4.15	0.00	0.00	0.00	27.32
SDC-6	(2)	26.96	2.86	21.53	13.41	0.00	0.00	0.00	0.70	0.00	0.93	0.00	5.79	5.94	0.00	0.00	0.00	21.89
SDC-7	(2)	23.41	2.48	21.14	21.67	0.00	0.00	0.00	0.94	0.00	0.96	0.00	7.93	7.09	0.00	0.00	0.00	14.37
SDC-8	(2)	20.00	2.12	17.50	28.08	0.00	0.00	0.00	0.91	0.00	0.97	0.00	7.20	6.13	0.00	0.00	0.00	17.11
SDC-9	(2)	19.41	2.06	16.74	19.28	0.00	0.00	0.00	0.87	0.00	14.91	3.14	0.00	4.54	0.00	0.00	0.00	19.05
SDC-10	(2)	18.49	1.96	13.29	15.62	0.00	0.00	0.00	0.67	0.00	13.64	17.31	0.00	0.00	0.00	0.00	1.58	17.44
SDC-11	(2)	19.65	2.08	14.26	15.89	0.00	0.00	0.00	0.74	0.00	14.66	7.69	0.00	3.31	0.00	0.00	0.00	21.71
SDC-12	(2)	24.45	2.59	17.69	11.30	0.00	0.00	0.00	0.78	0.00	9.61	14.21	0.00	0.00	0.00	0.00	2.25	17.12
SDC-13	(2)	22.17	2.35	17.19	7.17	0.00	0.00	0.00	0.54	0.00	7.29	8.50	0.00	0.00	0.00	0.00	14.58	20.21
SDC-18	(2)	0.85	0.09	5.73	15.79	0.00	0.00	0.00	0.59	0.00	8.40	4.39	0.00	0.00	0.00	0.00	22.00	42.17
SDC-19	(2)	26.97	2.86	10.66	13.63	0.00	0.00	0.00	0.63	0.00	10.25	6.24	0.00	0.00	0.37	0.00	0.00	28.39
SDC-20	(2)	8.78	0.93	9.32	24.60	0.00	0.00	0.00	0.76	0.00	20.35	9.97	0.00	0.00	0.44	0.00	0.00	24.84
SDC-21	(2)	30.96	3.28	19.66	7.79	0.00	0.00	0.00	0.45	0.00	6.45	7.30	0.00	0.00	0.70	0.00	0.00	23.41
SDC-22	(2)	27.00	2.86	9.26	12.52	0.00	0.00	0.00	0.82	0.00	9.83	11.33	0.00	0.00	0.00	0.00	1.23	25.15
SDC-23	(2)	7.74	0.82	3.39	23.41	0.00	0.00	0.00	0.64	0.00	8.64	12.53	0.00	0.00	0.00	0.00	7.31	35.52
SDC-24	(2)	18.11	1.92	7.49	24.77	0.00	0.00	0.00	0.87	0.00	9.82	0.00	1.32	5.36	0.00	0.00	0.00	30.34
SDC-25	(2)	29.41	1.88	17.74	6.98	0.00	0.00	0.00	0.65	0.00	0.00	0.00	1.83	5.56	0.00	0.00	0.00	35.96
SDC-26	(2)	16.72	1.77	16.00	14.90	0.00	0.00	0.00	0.76	0.00	10.98	0.00	4.36	5.36	0.00	0.00	0.00	29.15
SDC-27	(2)	13.00	1.38	24.11	24.97	0.00	0.00	0.00	0.82	0.00	9.44	0.00	4.48	7.92	0.00	0.00	0.00	13.87
SDC-28	(2)	22.12	2.35	21.02	12.65	0.00	0.00	0.00	0.81	0.00	12.18	0.00	2.11	6.06	0.00	0.00	0.00	20.69

Table 6. (Continued)

Sample number	#	ab	an	or	ill	klin	mnt	chl	rt	ap	dol	ank	srp	gt	sd	mgs	cal	qu
BS-2B	(4)	4.17	5.20	0.00	34.06	0.00	0.00	34.38	1.05	0.00	0.00	0.00	0.47	0.11	0.00	0.00	0.00	20.57
BS-2A	(3)	3.73	0.40	0.92	37.91	0.00	0.00	31.22	0.74	0.00	0.64	0.00	0.00	0.00	0.00	0.00	2.47	21.97
BS-1B	(3)	15.73	1.67	0.00	1.46	0.00	0.00	31.50	0.34	0.00	0.18	0.00	0.00	0.00	0.00	0.00	9.46	39.67
BS-1A	(5)	0.00	0.00	0.00	22.96	5.65	15.50	26.93	0.90	0.00	0.00	2.78	0.00	0.00	0.00	0.00	1.81	23.48
BS-3B	(4)	13.99	1.54	0.00	2.43	0.00	9.67	51.67	0.45	0.00	0.00	0.00	0.00	1.68	0.00	0.00	0.00	18.58
BS-3A	(4)	0.94	0.00	0.00	27.81	0.00	15.09	43.19	0.75	0.00	0.00	2.10	0.00	0.00	0.00	0.00	4.96	5.16
BS-10A	(2)	6.24	0.66	9.41	21.52	0.00	0.00	0.00	0.49	0.00	12.65	0.00	4.72	2.47	0.00	0.00	0.00	41.85
BS-10B	(2)	8.10	0.86	17.08	2.45	0.00	0.00	0.00	0.27	0.00	26.56	4.16	0.00	0.00	0.00	0.00	7.68	32.85
BS-15	(3)	0.85	0.09	1.63	0.00	0.00	0.00	75.56	0.15	0.00	7.99	1.27	0.00	0.00	0.00	0.00	7.83	4.63
BS-16A	(5)	0.00	0.00	0.00	7.49	3.38	0.00	0.00	0.17	0.00	0.00	0.38	0.00	2.76	0.00	0.00	0.00	85.82
BS-16B	(3)	0.29	0.03	6.10	0.00	0.00	0.00	82.93	0.17	0.00	1.99	0.73	0.00	0.00	0.00	0.00	5.63	2.13
M1A	(2)	36.42	3.86	7.56	7.39	0.00	0.00	0.00	0.62	0.00	2.79	8.50	0.00	0.00	0.00	0.00	7.81	25.05
M1B	(2)	32.20	3.42	8.83	10.21	0.00	0.00	0.00	0.61	0.00	5.18	11.35	0.00	0.00	0.00	0.00	3.02	25.19
M2A	(3)	7.44	0.79	2.57	6.53	0.00	0.00	52.43	0.34	0.00	0.00	0.11	0.00	0.00	0.00	0.00	6.30	23.50
M2B	(2)	15.23	1.62	1.32	18.96	0.00	0.00	0.00	0.68	0.00	4.42	7.93	0.00	0.00	0.00	0.00	2.54	47.29
M2D	(2)	20.07	2.13	12.30	21.81	0.00	0.00	0.00	0.37	0.00	3.61	6.02	0.00	0.00	0.00	0.00	4.61	29.08
M3	(2)	22.22	2.36	11.41	10.06	0.00	0.00	0.00	0.67	0.00	5.08	7.73	0.00	0.00	0.00	0.00	1.24	39.23

Minerals: See Table 3;

#Number of accepted calculation scheme according to Rosen and Nistratov (1984).

The comparison between observed (Table 5) and calculated (Table 6) compositions for arkoses and quartz arenites (Sangre de Cristo, Belden, and Maroon Formations) display higher but consistent discrepancies than those for the Uchur–Maya sandstones. Concentrations of quartz and plagioclase observed in the samples (Table 5) are in good agreement with the calculated norms. The observed potassic feldspar content are higher likely due to uncertainties in total matrix, cement and hematitic clay determination in thin sections as well as secondary sericite occurrence in potassic feldspar grains. Broad variations in calculated and observed carbonate (Tables 5 and 6) concentrations are in concordance and calculated norms seems to be more realistic, although it demands independent checking. These discrepancies are attributed mostly to uncertainties in opaques minerals determination in thin section.

Thus, calculated compositions for the Pennsylvanian to Lower-Permian arkoses and quartz arenites (Sandre de Cristo, Belden, and Maroon Formations) are about the same as observed in thin sections. These normative compositions suggest a more plagioclase-rich granitoid source and more intense weathering for the sandstones in the Belden Formation than in the Maroon and Sangre de Cristo formation that is in good agreement with geochemical data (Cullers, 2000).

CONCLUSION

The quantitative reconstruction (norm calculation) of the primary mineral composition of sedimentary and metasedimentary rocks should agree with the results of actual mineral compositions of the investigated rocks (using modal, X-ray or statistically representative microprobe analyses). Disagreement between the norms and modes may arise with an increase in the amount of unknown minerals in the matrix and cement of the rocks or because of the lack of minerals in the normative calculation. The latter is due to the norms in sedimentary rocks being calculated from an ordered mixture of primary and secondary minerals from the accepted basis. The authors express his gratitude to Dr S. Henley for valuable remarks and proof reading of the paper. RLC thanks the crew of the nuclear reactor of Kansas State University for irradiating the samples and for use of their equipment.

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APPENDIX: SEQUENCE OF NORM CALCULATION

The set of basic minerals is represented in this table as molecular proportions of oxides in each mineral

	SiO ₂	TiO ₂	Al ₂ O ₃	FeO ^a	MnO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅
Qu	1	0	0	0	0	0	0	0	0	0
Ab	6	0	1	0	0	0	0	1	0	0
An	2	0	1	0	0	0	1	0	0	0
Or	6	0	1	0	0	0	0	0	1	0
Ill	16	0	6.5	1	0	1	0	0	2	0
Kln	2	0	1	0	0	0	0	0	0	0
Mnt	24	0	5	0	0	2	0	1	0	0
Chl	1	0	1	1	0	1	0	0	0	0
Rt	0	1	0	0	0	0	0	0	0	0
Ilm	0	1	0	1	0	0	0	0	0	0
Gt	0	0	0	1.1	0	0	0	0	0	0
Cal	0	0	0	0	0	0	1	0	0	0
Dol	0	0	0	0	0	1	1	0	0	0
Sd	0	0	0	1	0	0	0	0	0	0
Ank	0	0	0	1	0	0	1	0	0	0
Mgs	0	0	0	0	0	1	0	0	0	0
Srp	2	0	0	0	0	3	0	0	0	0
Ap	0	0	0	0	0	0	3	0	0	1

^aTotal Fe as FeO.

where Qu – quartz (SiO₂); Ab – albite (Na₂O, Al₂O₃, 6SiO₂); An – anortite (CaO, Al₂O₃, 2SiO₂); Or – orthoclase (K₂O, Al₂O₃, 6SiO₂); Ill – illite (2K₂O, FeO, MgO, 6.5Al₂O₃, 16SiO₂); Kln – kaolinite (Al₂O₃, 2SiO₂); Mnt – montmorillonite (Na₂O, 2MgO, 5Al₂O₃, 24SiO₂); Chl – chlorite (FeO, MgO, Al₂O₃, SiO₂); Rt – rutile (TiO₂); Ilm – ilmenite (FeO, TiO₂); Gt – goethite (1.1FeO); Cal – calcite (CaO); Dol – dolomite (CaO, MgO); Sd – siderite (FeO); Ank – ankerite (FeO, CaO); Mgs – magnesite (MgO); Srp – serpentine (3MgO, 2SiO₂); Ap – apatite (3CaO, P₂O₅).

The consequent stages of mineral subtraction (after Rosen and Nistratov, 1984)

- I. Determination of rock type using Al/other elements ratios according to the first column in Table 1 (Rosen and Nistratov, 1984).
- II. Subtraction of Rt and Ap from a sample, exploring TiO_2 and P_2O_5 content.
- III. Subtraction of minerals according to the type of rock:
 - 1). Type 1 : Ab + An; Or;
 - 2). Type 2 : Ab + An; Or + Ill;
 - 3). Type 3 : Ab + An; Or + Ill + Chl;

In cases 2) and 3) if $\text{CaO} > 0.2 \text{Na}_2\text{O}$ (in molar quantities, as accepted for plagioclase formula), for subtraction is used CaO molar content equal $0.2 \text{Na}_2\text{O}$.

- 4). Type 4 : Ill; Ab + An + Mnt + Chl
- 5). Type 5 : Ill + Mnt + Chl; Kln
- IV. The remnants of oxides are distributed among other minerals from the set accordingly to the scheme in Table 2 in Rosen and Nistratov (1984).