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DISCRIMINANT ANALYSIS OF CLAY MINERAL COMPOSITIONS

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Abstract—Compositional data for 464 clay minerals (2:1 type) were analyzed by statistical techniques. The objective was to understand the similarities and differences between the groups and subgroups and to evaluate statistically clay mineral classification in terms of chemical parameters. The statistical properties of the distributions of total layer charge (TLC), K, ^{VI}Al, ^{VI}Mg, octahedral charge (OC) and tetrahedral charge (TC) were initially evaluated. Critical-difference (P = 1%) comparisons of individual characteristics show that all the clay micas (illite, glauconite and celadonite) differ significantly from all the smectites (montmorillonite, beidellite, nontronite and saponite) only in their TLC and K levels; they cannot be distinguished by their ^{VI}Al, ^{VI}Mg, TC or OC values which reveal no significant differences between several minerals.

Linear discriminant analysis using equal prior was therefore performed to analyze the combined effect of all the chemical parameters. Using six parameters [TLC, K, ^{VI}Al, ^{VI}Mg, TC and OC], eight minerals groups could be derived, corresponding to the three clay micas, four smectites (mentioned above) and vermiculite. The fit between predicted and experimental values was 88.1%. Discriminant analysis using two parameters (TLC and K) resulted in classification into three broad groups corresponding to the clay micas, smectites and vermiculites (87.7% fit). Further analysis using the remaining four parameters resulted in subgroup-level classification with an 85–95% fit between predicted and experimental results. The three analyses yielded D^2 Mahalanobis distances, which quantify chemical similarities and differences between the broad groups, within members of a subgroup and also between the subgroups. Classification functions derived here can be used as an aid for classification of 2:1 minerals.

Key Words—Classification, Correlations, Critical Difference, Discriminant Analysis, Kurtosis, Micas, Skewness, Smectites, Statistical Analysis, Vermiculites.

INTRODUCTION

Clay minerals have complex compositions which are defined by several chemical parameters having a range of values that often overlap between the different types. This presents difficulties in classification and in understanding their compositional differences, particularly with closely related mineral types. Crystallographic properties provide a fairly reliable means of differentiating the major clay mineral groups, *i.e.* smectites, clay micas, vermiculites, chlorites and kaolinites. Problems arise at the second level (the subgroup level) where differences are mainly chemical, *e.g.* differentiating between montmorillonite, beidellite, saponite, *etc.* (Newman and Brown, 1987; Reider *et al.*, 1998). This problem has, therefore, been approached from various angles. Schultz (1969) used several parameters including Li-test and thermal characteristics to distinguish between montmorillonite and beidellite groups. Grim and Kulbicki (1961) using chemical and other data concluded that montmorillonite does not form a single continuous series. Ternary phase diagrams were used by Vogt and Köster (1978) to differentiate between montmorillonite, beidellite and nontronite. Velde (1985) showed from chemical and phase equilibria studies that illite and glauconite are distinct species and that the latter is not a subspecies of illite. Brigatti and Poppi (1981) used Q-mode multivariate analysis to distinguish between the dioctahedral smectites. Another approach has been the use of fuzzy logic to analyze the vagueness in clay compositions and to quantify the compositional overlap between the mineral types (Varadachari *et al.*, 2003).

Discriminant analysis, also known as 'statistical pattern recognition', is a statistical technique (Seber, 1984) used popularly in the classification of biological materials. In this technique, various analyses can be performed, given g distinct groups in a population P having d measured characteristics x associated with it. Thus, in the case of clay minerals, it can be used to (1) evaluate the relevance of the groups g, (2) study the distances between the groups, and (3) choose the number of chemical parameters d and the characteristic type x which best differentiate the groups. Application of linear discriminant analysis could, therefore, provide new insights regarding the compositions of clay minerals.

In this work, we have used this statistical technique to analyze the chemical compositions of a large number of clay minerals. Initially, the differences between the individual chemical parameters in the various types of clays have been studied. This brings out clearly the parametric factors distinguishing closely related species and also those chemical factors, which for two species are indistinguishable. Discriminant analysis was carried out to evaluate the combined effect of the major chemical parameters. It is seen how clay minerals can

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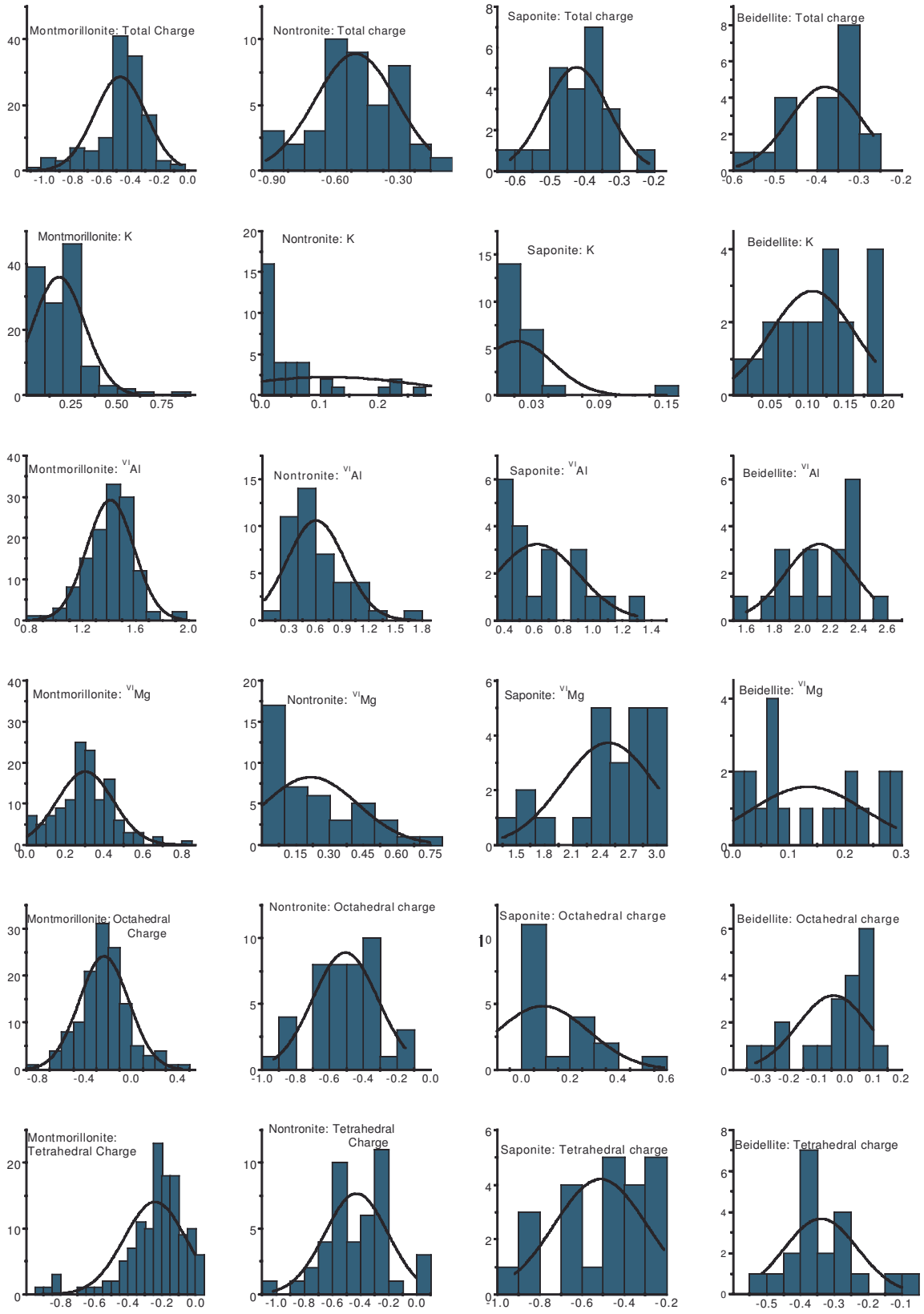

Figure 1. (*this and facing page*) Histograms and normal curves showing distributions of chemical parameters in the clay minerals.

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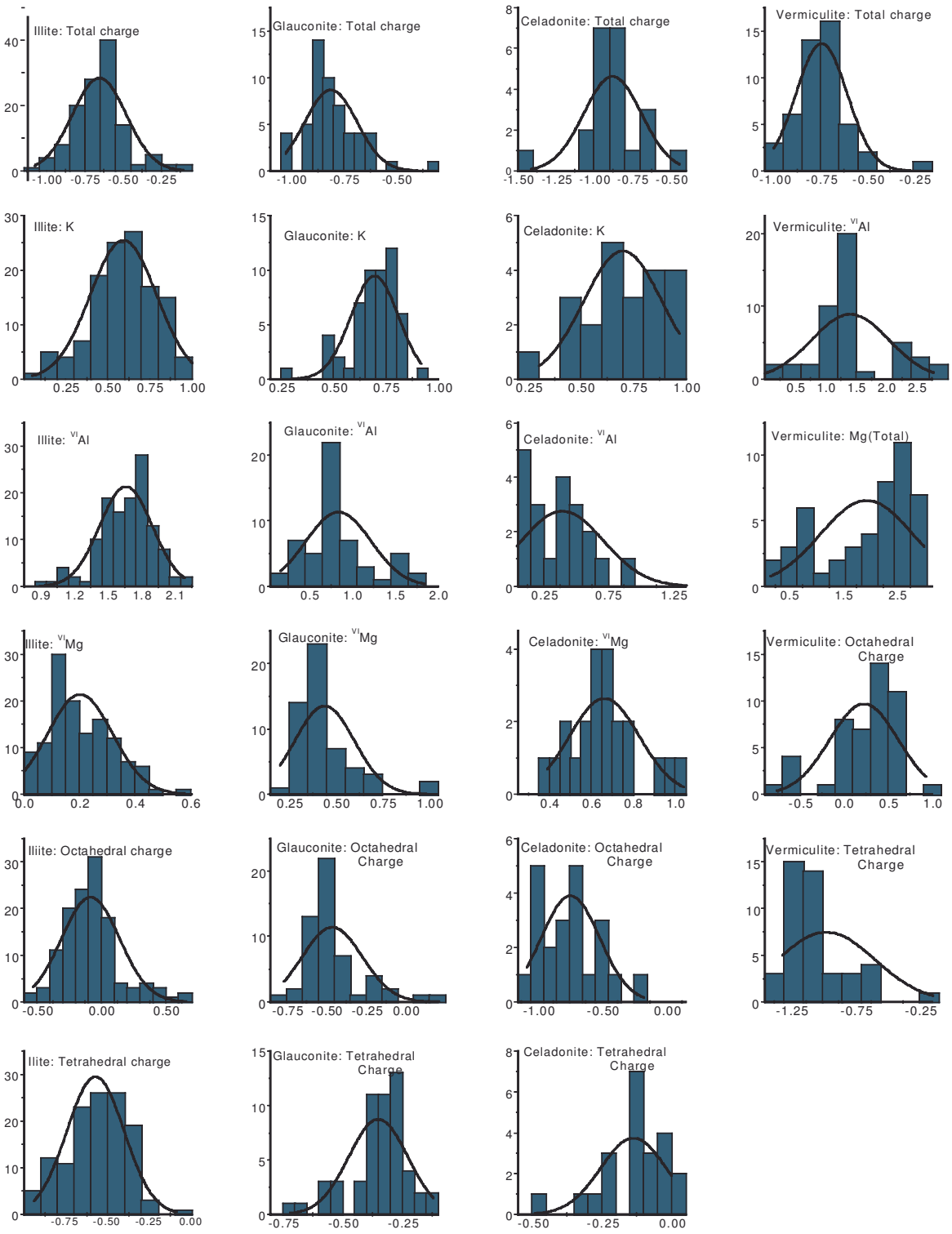

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be distinguished chemically from each other forming chemically distinct groups. Distances between the mineral compositions have been evaluated to show the degree of separation between the groups. It is also possible to select the parameters for distinguishing clay subgroups. Classification functions have been derived so that discriminant analysis can be used as a supporting tool for classifying or identifying clay minerals on the basis of their chemical composition data.

METHODOLOGY

Chemical composition data for 2:1 clay minerals (464 minerals in all) were collected from the literature and are available in Varadachari *et al.* (2003) as electronic supplementary material [http://dx.doi.org/10.1007/s00114-002-0387-y]. The minerals include smectites, clay micas and vermiculites. To maintain charge neutrality in the formulae, minor adjustments were necessary in some instances. (For example, an excess negative charge of 0.002 is balanced by increasing exchangeable Ca^{2+} by 0.001 and *vice versa*). Formulae are expressed in terms of the major ions Si, ^{IV}Al, ^{VI}Al, ^{VI}Mg, Fe^{2+}, Fe^{3+}, K, Na, Ca, Mg (exchangeable), O and OH; trace ions such as F, Mn or Zn were adjusted by equivalent amounts of OH^-, Fe^{2+} or Mg^{2+}.

Distributions of the major chemical parameters were represented as histograms and normal curves. Dispersion of the data was evaluated as the standard deviation. As an observation of the nature of the frequency distributions of the compositional parameters, skewness and kurtosis values were also determined. To compare the significance of the differences in chemical constituents between mineral types, the F statistic test was applied. The significance of the differences between the means of the parameters was evaluated from the critical difference (CD) values. General discriminant analysis using equal prior (giving equal weightage to all parameters) was carried out on all 464 minerals. A standard linear classification function was chosen as being suitable to the characteristics of the data set on the basis of fundamental statistical principles. The variables (chemical parameters) include total layer charge (TLC), K, tetrahedral charge (TC), octahedral charge (OC), ^{VI}Al and ^{VI}Mg contents. The analysis was performed using (1) all six chemical parameters (mentioned above) for classification at the subgroup level, (2) two chemical parameters (TLC and K content) for classification at the broad group level followed by four different parameters [TC, OC, ^{VI}Mg and ^{VI}Al] for subgroup level classification. The Mahalanobis D-squared measure of the distances between the groups and subgroups were also evaluated. Samples, reclassified statistically, were compared with the original classification to analyze the deviations. Computations were carried out using the 'Statistica' software (program for general discriminant analysis using equal prior).

RESULTS AND DISCUSSION

Histograms showing total layer charge (TLC), K, tetrahedral charge (TC), octahedral charge (OC), ^{VI}Al and ^{VI}Mg distributions, together with fitted normal curves are shown in Figure 1. Skewness of the curves as well as the kurtosis values are given in Table 1. Symmetrical distributions with skewness close to zero are observed for many parameters including TLC of nontronite, saponite, illite and celadonite, K levels in beidellite, illite and celadonite, ^{VI}Mg levels in most minerals, *etc.* Kurtosis values close to ideal (*i.e.* 0) are seen in TLC values for nontronite, saponite, beidellite, OC of saponite, beidellite, celadonite, TC of nontronite, beidellite, illite, *etc.*

Mean values and standard deviations of the distributions can be seen in Table 1. The significance of the critical differences between the means were evaluated at the 1% level and are also given in Table 1. The results show that the minerals of the smectite group (montmorillonite, beidellite and saponite) do not differ significantly in their TLC. Similarly, differences in values of TLC for celadonite and glauconite are not significant. All subgroups of the clay micas (illite, glauconite and celadonite) have, as expected, significantly higher K levels than those of the smectite group (montmorillonite, beidellite, saponite and nontronite). However, for the other four parameters [TC, OC, ^{VI}Al and ^{VI}Mg], the differences between the smectite group and the clay mica group are not unequivocal. For example, critical differences at 1% level (t-test) shows that (1) there is no significant difference in the average tetrahedral charges of montmorillonite-celadonite, glauconite-nontronite and illite-saponite, (2) illite, nontronite and beidellite have statistically similar octahedral charges, (3) ^{VI}Al levels are not significantly different in illite-beidellite and nontronite-celadonite, and (4) beidellite-illite-nontronite have similar Mg levels.

Correlations between various compositional parameters were also studied (Table 2). High correlations between TLC and K levels are seen for illites and glauconites but are much less for celadonites. A fair correlation (0.4–0.5) is also shown by all minerals of the smectite group, except saponite. In celadonites and glauconites, TLC and OC are highly correlated; therefore, in these minerals, increasing TLC is largely due to increasing OC. For all other minerals, except saponite and vermiculite, correlations are in the medium range. Relationships between TLC and TC are, however, poor in all minerals except nontronite and saponite (Table 2). Thus, changes in TLC of minerals appear to be more influenced by the OC than by the TC. The ^{VI}Al-^{VI}Mg correlations suggest that ^{VI}Mg is substituted at the expense of ^{VI}Al in illite and beidellite. Correlations with Fe^{3+} levels were also evaluated here; Fe^{3+} shows an increase at the expense of ^{VI}Al in beidellite, illite, glauconite and celadonite as seen from the high negative

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Table 1. Distributions of various chemical parameters in clay minerals.

Mineral	Parameters	Skewness	Kurtosis	Standard deviation	Mean	Parameters	Significance of differences at p = 1%*
Montmorillonite (M)	TLC	−1.03	1.50	0.180	−0.473	TLC	C G V I N M S B
	K	1.36	4.23	0.143	0.179		
	^{VI}Al	−1.12	4.66	0.199	1.41		
	^{VI}Mg	0.312	1.07	0.144	0.302		
	OC	0.214	1.03	0.213	−0.234		
	TC	−1.581	3.234	0.183	−0.234		
Nontronite (N)	TLC	−0.35	−0.205	0.193	−0.506	K	V S B N M I G C
	K	1.54	1.80	0.152	0.114		
	^{VI}Al	1.44	1.44	0.275	0.196		
	^{VI}Mg	0.847	−0.225	0.208	0.216		
	OC	0.347	1.22	0.237	−0.078		
	TC	−0.271	0.287	0.224	−0.428		
Saponite (S)	TLC	−0.06	0.344	0.091	−0.423	^{VI}Al	S N C V G M I B
	K	3.56	14.57	0.032	0.017		
	^{VI}Al	2.75	8.66	0.185	0.107		
	^{VI}Mg	−1.16	0.463	0.484	2.483		
	OC	0.810	0.694	0.190	0.088		
	TC	−0.375	−1.012	0.219	−0.512		
Beidellite (B)	TLC	−0.99	0.469	0.087	−0.38	^{VI}Mg	B I N M G C V S
	K	−0.219	−0.789	0.056	0.106		
	^{VI}Al	−1.08	0.120	0.207	1.78		
	^{VI}Mg	0.231	−1.51	0.101	0.133		
	OC	−1.083	−0.103	0.126	−0.042		
	TC	0.771	0.466	0.108	−0.339		
Illite (I)	TLC	0.494	1.26	0.177	−0.655	OC	C G M I N B S V
	K	−0.342	0.269	0.198	0.594		
	^{VI}Al	−0.623	0.829	0.236	1.66		
	^{VI}Mg	0.416	−0.209	0.118	0.203		
	OC	0.910	1.53	0.225	−0.083		
	TC	−0.174	−0.321	0.170	−0.573		
Glauconite (G)	TLC	1.08	2.63	0.124	−0.81	TC	V I S N G B M C
	K	−1.05	1.782	0.114	0.700		
	^{VI}Al	0.573	−0.182	0.318	0.512		
	^{VI}Mg	1.90	4.22	0.160	0.440		
	OC	1.63	3.44	0.189	−0.456		
	TC	−0.945	1.335	0.123	−0.35		
Celadonite (C)	TLC	−0.361	2.65	0.19	−0.877		
	K	−0.520	−0.507	0.187	0.701		
	^{VI}Al	1.15	0.746	0.248	0.259		
	^{VI}Mg	0.592	0.295	0.166	0.857		
	OC	0.687	0.377	0.226	−0.736		
	TC	−1.452	2.782	0.117	−0.136		
Vermiculite (V)	TLC	1.12	3.72	.138	−0.743		
	K	–	–	–	0.00		
	^{VI}Al	1.33	0.484	0.533	0.436		
	^{VI}Mg	−0.750	−0.826	0.857	1.94		
	OC	−1.11	0.89	0.388	0.228		
	TC	1.662	1.870	0.376	−0.971		

TLC: total layer charge, TC: tetrahedral charge, OC: octahedral charge
* minerals connected by lines (underlined or overlined) do not differ significantly

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Table 2. Correlations between various chemical parameters.

Mineral	Correlation coefficients for						
	TLC-K	TLC-OC	TLC-TC	TC-OC	^{VI}Al-^{VI}Mg	^{VI}Al-Fe^{3+}	^{VI}Mg-Fe^{3+}
Montmorillonite	−0.54	0.58	0.31	−0.3	−0.33	−0.23	−0.23
Nontronite	−0.47	0.47	0.50	−0.65	−0.08	−0.42	−0.60
Saponite	0.01	−0.10	0.50	−0.91	−0.27	0.24	−0.39
Beidellite	−0.46	0.53	0.18	−0.74	−0.65	−0.74	0.42
Illite	−0.97	0.66	0.16	−0.63	−0.80	−0.83	0.45
Glauconite	−0.81	0.76	−0.16	−0.76	−0.46	−0.79	0.12
Celadonite	−0.42	0.85	−0.02	−0.54	−0.08	−0.71	−0.44
Vermiculite	#	0.26	0.10	−0.94	−0.58	−0.18	−0.25

Indeterminable (divisor zero)

correlations. Fe^{3+} substitution for ^{VI}Mg is generally poor except in nontronite. The TC and OC appear to share an inverse relationship. This negative correlation is highest in saponite and vermiculite followed by glauconite and beidellite. The only exception is montmorillonite, which does not reveal any interdependence between the charges.

The results of discriminant analysis of the 464 (2:1 structural type) minerals in the eight clay subgroups, using six parameters, are shown in Table 3. The linear classification matrix, squared Mahalanobis distances between the subgroups, and classification functions for identification are also given in Table 3. The following inferences may drawn:

(1) The statistically derived eight classes that correspond to the eight subgroups show significant differences in their chemical compositions. The various clay minerals are, therefore, distinctly different from one another. It may be recalled, that if the chemical parameters are compared individually (Table 1) there is much overlapping of the data and the minerals cannot be differentiated distinctly (Table 2). However, on combining the six parameters, the overall differences in the mineral compositions are evident (Table 3).

(2) The squared Mahalanobis distances between the mineral subgroups, as shown in Table 3, are all highly significant (at probability levels <0.0001%). The data may be interpreted as follows: montmorillonite is equally distant from nontronite and saponite but is closer to beidellite. Illite is chemically closest to beidellite (D^2 = 13.7). Glauconite and celadonite have a very small distance separation (3.1) but are nevertheless chemically distinct. Vermiculites are closest to saponites.

(3) Experimental (original) groupings of the minerals when compared with the groupings predicted from discriminant analysis show a high degree of matching between the two; after statistical classification, 88% of the minerals fit into the same group to which they were originally assigned. Thus, out of 129 samples experimentally classified as montmorillonites, 115 samples statistically fall within this group whereas 14 appear to be more beidellitic. All 20 samples of beidellite are estimated as belonging to this subgroup. Similarly, out of 126 experimentally classified illites, 112 of them fit into this group, 11 samples are classified as beidellites and three as glauconites.

To optimize the parameters for describing clay mineral groups and subgroups and obtain the best fit of observed and predicted classifications, a two-level approach was attempted. Initially, the minerals were classified as broad groups, *i.e.* smectites, clay micas and vermiculites, on the basis of two chosen variables (total layer charge and K content). Subsequently, each broad group was further classified using four other variables, *i.e.* tetrahedral charge, octahedral charge, ^{VI}Al and ^{VI}Mg.

Table 4 shows the results of the first level of classification of the 464 minerals into three broad groups. Three broad groups can be clearly defined using two variables together (total charge and K content). There is an 87.7% fit between the observed and predicted classifications. This is significant at the 0.33% probability level. Squared Mahalanobis distances between the groups (Table 4) are also highly significant (p <0.0001%). It may be observed that the distance between clay mica and smectite is smaller (11.0) than that between clay mica and vermiculite (32.9) and smectite is almost equally distant from the clay mica and vermiculite groups. Classification functions given in Table 4 may be used for evaluating the broad group of an unknown sample.

The results of the second level of classification of the minerals into subgroups are shown in Table 5. With the clay micas, the fit between experimental and predicted classification is 86.1%. Some glauconites appear in the celadonite and illite groups. The distance between glauconite-illite and glauconite-celadonite being fairly close, with borderline samples, there could have been some error in the original classification of these minerals. The Mahalanobis distances given in Table 5 show the separations between the minerals at the subgroup level unlike Table 3, which gives the overall distances (including both group and subgroup).

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Table 3. Classification matrix, Mahalanobis distances and classification functions with six variables.

Observed classification		Predicted classification							
Class	% correct	1 p = 0.125	2 p = 0.125	3 p = 0.125	4 p = 0.125	5 p = 0.125	6 p = 0.125	7 p = 0.125	8 p = 0.125
1	89.1	115.0	0.00	14.0	0.00	0.00	0.00	0.00	0.00
2	90.7	0.00	39.0	2.00	0.00	0.00	2.00	0.00	0.00
3	100.0	0.00	0.00	20.0	0.00	0.00	0.00	0.00	0.00
4	95.6	0.00	0.00	1.00	22.0	0.00	0.00	0.00	0.00
5	88.9	0.00	0.00	11.0	0.00	112.0	3.00	0.00	0.00
6	79.6	0.00	0.00	0.00	0.00	4.00	43.0	7.00	0.00
7	86.4	0.00	1.00	0.00	0.00	0.00	2.00	19.0	0.00
8	83.0	0.00	1.00	4.00	3.00	0.00	0.00	0.00	39.0
Total	88.1	115.0	41.0	52.0	25.0	116.0	50.0	26.0	39.0

	Squared Mahalanobis distances							
Class	1	2	3	4	5	6	7	8
1	0.00	69.4	14.1	70.2	30.2	44.4	43.4	71.9
2	69.4	0.00	59.8	102.6	69.8	29.3	35.7	74.9
3	14.1	59.8	0.00	68.5	13.7	39.1	45.0	57.3
4	70.2	102.6	68.5	0.00	86.8	82.4	73.0	21.9
5	30.2	69.8	13.7	86.8	0.00	23.2	33.3	73.7
6	44.4	29.3	39.1	82.4	23.2	0.00	3.1	74.9
7	43.4	35.7	45.0	73.0	33.3	3.1	0.00	74.8
8	71.9	74.9	57.3	21.9	73.7	74.9	74.8	0.00

All values significant at p <0.0001%

	Classification functions							
Effect	1 p = 0.28	2 p = 0.09	3 p = 0.04	4 p = 0.05	5 p = 0.27	6 p = 0.12	7 p = 0.05	8 p = 0.10
Intercept	−27.5	−12.4	−45.0	−59.2	−36.5	−28.3	−28.4	−71.9
TLC	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	−3.32	−14.2	−2.23	−16.5	23.6	21.5	17.2	−32.4
^{VI}Al	27.9	9.51	37.2	27.3	29.3	20.6	17.8	31.8
^{VI}Mg	15.4	5.83	18.2	36.2	14.3	12.6	13.6	32.4
OC	−29.0	−29.0	−27.9	−31.3	−18.2	−23.2	−28.4	−52.9
TC	−9.74	−28.8	−4.45	−17.1	−5.70	−10.8	−12.2	−45.1

Note: 1 – montmorillonite; 2 – nontronite; 3 – beidellite; 4 – saponite; 5 – illite; 6 – glauconite; 7 – celadonite; 8 – vermiculite

Classification functions listed in Table 5 may be used for identifying unknown samples, which have already been classified into the clay mica broad group by XRD methods or by the statistical technique mentioned above.

Discriminant analysis of the smectite subgroup gives an excellent fit (95.3%) between observed and predicted classifications. Of the 129 montmorillonites, 124 are found within this group and only five appear in other subgroups. Similarly, only two nontronites, two beidellites and one saponite are predicated as being misclassified. All subgroups differ significantly from each other when judged by the four chemical parameters. Saponites are farthest from montmorillonites as well as beidellites and nontronites. Beidellites and montmorillonites are the closest pair. Derived classification functions, for identification of unknown samples are shown in Table 5. This may be used for samples otherwise identified as smectites (by XRD or other techniques). The probability error in such classification would be as shown in Table 5.

SUMMARY AND CONCLUSIONS

The chemical compositions of 464 clay minerals were analyzed statistically to determine the differences between the mineral groups and subgroups and to evaluate the relevance of the classification in terms of the chemical parameters. All members of the smectite group (montmorillonite, nontronite, beidellite and saponite) differ significantly from the members of the clay mica group (illite, glauconite and celadonite) in their total charge and K levels; however, with other chemical

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Table 4. Classification matrix, distances and classification functions for broad group analysis with two variables.

Observed classification		Predicted classification			Class	Squared Mahalanobis distances			Effect	Classification functions		
Class	% correct	1 $p = 0.33$	2 $p = 0.33$	3 $p = 0.33$		1	2	3		1 $p = 0.44$	2 $p = 0.46$	3 $p = 0.10$
1	90.6	183.0	17.0	2.00	1	0.00	11.0	32.9	Intercept	−10.8	−5.07	−19.3
2	82.8	9.00	178.0	28.0	2	11.0	0.00	10.1	TLC	−14.1	−21.8	−45.7
3	97.9	0.00	1.00	46.0	3	32.9	10.1	0.00	K	15.3	−11.1	−35.6
Total	87.7	192.0	196.0	76.0								

Note: 1 – clay mica, 2 – smectite, 3 – vermiculite

parameters, there is much overlap between the mineral groups. Thus, illite and saponite have statistically similar tetrahedral charges; so do glauconite and nontronite. Other chemical parameters which do not differ significantly are, octahedral charges, ^{VI}Al and ^{VI}Mg levels in illite and beidelite, ^{VI}Al levels in nontronite and celadonite, *etc.* Individual chemical components, therefore, cannot be used for distinguishing clay groups and subgroups.

An attempt was made to analyze the total effect of these differences which might reveal whether each type of clay mineral is indeed different from the other in terms of its major chemical parameters. Linear discriminant analysis was therefore carried out to evaluate the combined effect of the chemical factors. Initially, discriminant analysis using six chemical parameters showed that the 464 minerals could be successfully divided into eight distinct classes with an excellent fit between the predicted and observed classifications. Derived Mahalanobis distances provide a measure of the overall separations between each mineral type. Thus, some of the overall distances between the minerals are, illite–celadonite = 33.3, glauconite–celadonite = 3.1, montmorillonite–beidellite = 14.1, illite–beidellite = 13.7, nontronite–glauconite = 29.3.

At the next stage, the 464 minerals were classified into broad groups using two variables, *i.e.* total layer charge and K levels. The results showed that the broad groups, smectite, clay mica and vermiculite, could be clearly differentiated by only these two chemical parameters taken together. Statistically predicted classification of clay minerals into broad groups shows excellent agreement with experimental observations. Squared Mahalanobis distances between the groups are highly significant and reaffirm the observation that clay mineral groups can be satisfactorily distinguished using the two chemical parameters, TLC and K content.

Each of the groups was further divided into subgroups using the four other chemical parameters, *i.e.* tetrahedral charge, octahedral charge, ^{VI}Al and ^{VI}Mg. With the combined effect of these four parameters, every subgroup mineral differed significantly from every other subgroup mineral. Matching between predicted and experimental classifications is ~85–95%. Mahalanobis distances between the subgroups are also highly significant. Thus, illites, glauconites and celadonites are chemically distinguished, as are montmorillonites, nontronites, beidellites and saponites. Discriminant analysis, therefore, reveals that in spite of their many similarities, the clay minerals are chemically distinct and different.

Mineral classification functions derived here may be utilized for classifying an unknown sample into its broad group and subgroup. It could also be used as an additional tool for evaluating doubtful cases of mineral identification.

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Table 5. Classification matrix, squared Mahalanobis distances and classification functions for subgroup analysis with four variables.

(A) Smectite group

Classification matrix						Squared Mahalanobis distances					Classification functions				
Observed classification		Predicted classification													
Class	% correct	1 p = 0.25	2 p = 0.25	3 p = 0.25	4 p = 0.25	Class	1	2	3	4	Effect	1 p = 0.6	2 p = 0.2	3 p = 0.09	4 p = 0.11
1	96.1	124.0	3.00	2.00	0.00	1	0.00	17.8	9.49	116.1	Intercept	−28.7	−11.3	−53.0	−85.8
2	95.3	2.00	41.0	0.00	0.00	2	17.8	0.00	49.2	118.0	^{VI}Al	31.8	12.8	45.1	21.4
3	90.0	2.00	0.00	18.0	0.00	3	9.49	49.2	0.00	148.9	^{VI}Mg	11.8	6.98	11.4	58.3
4	95.6	1.00	0.00	0.00	22.0	4	116.1	118.0	148.9	0.00	OC	−21.2	−16.8	−19.7	−6.2
Total	95.3	129.0	44.0	20.0	22.0						TC	−12.8	−20.4	−10.0	−19.1

Note: 1 – montmorillonite, 2 – nontronite, 3 – beidellite, 4 – saponite

(B) Clay mica group

Classification matrix					Squared Mahananobis distance				Classification functions			
Observed classification		Predicted classification										
Class	% correct	5 p = 0.62	6 p = 0.27	7 p = 0.11	Class	5	6	7	Effect	5 p = 0.62	6 p = 0.27	7 p = 0.11
5	95.2	120.0	6.00	0.00	5	0.00	8.12	21.0	Intercept	−49.2	−39.3	−42.7
6	72.2	9.00	39.0	6.00	6	8.12	0.00	3.71	^{VI}Al	39.3	30.2	28.3
7	68.2	1.00	6.00	15.0	7	21.0	3.71	0.00	^{VI}Mg	46.5	48.4	56.3
Total	86.1	130.0	51.0	21.0					OC	−37.2	−37.6	−38.1
									TC	−34.3	−34.3	−29.7

Note: 5 – illite, 6 – glauconite, 7 – celadonite

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APPENDIX

This is an example to illustrate how a mineral of a known chemical composition (chemical formula) could be classified. Assume that the sample to be studied has the formula $Si_{3.93}{}^{IV}Al_{0.07}{}^{VI}Al_{1.495}Fe^{3+}_{0.145}Mg_{0.36}Na_{0.425}K_{0.005}O_{10}(OH)_2$; the values for the chemical parameters are, therefore, TLC = −0.43, K = 0.005, ^{VI}Al = 1.495, ^{VI}Mg = 0.36, TC = −0.07, OC = −0.36 (Camp Berteau montmorillonite from Newman and Brown, 1987). The equation for the linear classification function (LCF) for clay mica broad group is $P_i = a_i x + b_i y + c_i$, where P_i is the classification score for the i^{th} broad group, a_i and b_i are the values of the classification constants for TLC and K respectively, c_i is the intercept and x and y are the actual values for TLC and K for the mineral. On substituting the constants for the equation from Table 4, we have the LCF, $P_1 = -10.8 - 14.1x + 15.3y$; for our sample x = −0.43 and y = 0.005; therefore, the classification score $P_1 = -4.66$. Similarly, we obtain probability functions $P_2 = 4.25$ and $P_3 = 0.17$ (for smectite and vermiculite broad groups, respectively). Since the classification score, P_2, is largest, the mineral is assigned to the smectite broad group.

Similarly, at the subgroup level, the equation for the linear classification function is $S_j = m_j q + n_j r + o_j s + p_j t + u_j$, where m_j, n_j, o_j and p_j are the classification constants for ^{VI}Al, ^{VI}Mg, TC and OC respectively, p_j is the intercept, and q, r, s and t are the observed values of these chemical parameters in the sample. Utilizing the classification constants in Table 5, the derived classification scores, S_1, S_2, S_3 and S_4 for the smectite subgroups, montmorillonite, nontronite, beidelite and saponite are 31.62, 17.83, 26.32 and −29.25 respectively. The mineral, therefore, is assigned to the highest density subgroup, montmorillonite.