

## POTASSIUM- AND AMMONIUM-TREATED MONTMORILLONITES. II. CALCULATION OF CHARACTERISTIC LAYER CHARGES

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**Abstract**—The formation of an interstratified structure in dioctahedral smectite was assumed to be influenced by (1) the overall layer charge density and its distribution in the structure, (2) the solvation energy of the cation, and (3) the nature of the solvation agent. By holding factors (2) and (3) constant it was possible to calculate the average local charge densities  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$  which are necessary for formation of 10-, 14-, and 16.8-Å mixed-layer phases in potassium-treated and ethylene glycol (EG) saturated smectites. The values of  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$  were 1.99, 1.2, and 0.56 esu/unit cell, respectively. Ammonium-treated smectites saturated with EG gave corresponding mean local charge densities of 2.7, 1.6, and 0.72 esu/unit cell. Calculations were made under the limiting condition  $QA > QC > QE > 0$ .

For K-smectites saturated with EG,  $Q_{tot} = 1.99pA + 1.2pC + 0.56pE$ , where  $Q_{tot}$  is the total charge (esu/unit cell), and pA, pC, and pE are probability coefficients for 10-, 14-, and 16.8-Å phases in the interstratified structure. The above equation calculated with the aid of least squares and without the limiting condition yields

$$Q_{tot} = 2.05pA + 1.29pC + 0.33pE.$$

There is a good agreement between values obtained for K-smectites and those for mica, vermiculite, and montmorillonite layer charges for which the above unit-structure distances are typical.

**Key Words**—Ethylene glycol complex, Interstratification, Layer charge, Mixed layer, Montmorillonite.

### INTRODUCTION

Various authors have proved the existence of two and three kinds of unit structures in smectites saturated with monovalent ions with low solvation energy, such as  $K^+$ ,  $NH_4^+$ ,  $Rb^+$ , and  $Cs^+$  (Dyal and Hendricks, 1952; Weaver, 1958; Tettenhorst and Johns, 1966; Sawhney, 1969; Shutov *et al.*, 1969; Muravyov and Sakharov, 1970). Such behavior is quite common (Číčel and Machajdík, 1981), and at present it is accepted that the formation of mixed-layer structures is caused by different local layer charges of smectites.

Collapse of the interlayer of smectite is determined by interaction of the cation hydration energy and the electrostatic force between the negative layer charge and cation. Wear and White (1951), Weaver (1958), and Mackenzie (1963) suggested that the decisive factor influencing the collapse of smectites is the nature of the charge located on the tetrahedral sheet. Tettenhorst and Johns (1966) and Drits (1966) emphasized that the tetrahedral charge ought to be located symmetrically on both sides of the interlayer space, if a collapse to 10 Å is to take place. Others, such as Weir (1965), Schultz (1969), Sawhney (1969), and Horváth and Novák (1976), claimed that the total charge of the unit cell is the controlling factor.

The variability of the local layer charges of smectite has been assumed explicitly by various authors, but the method of determination of charge distribution appeared only in recent years (e.g., Lagaly and Weiss,

1969; Lagaly *et al.*, 1976; Stul and Mortier, 1974). The total layer charge was presented as an average value. If the layer charge is responsible for the contractibility of the smectite interlayers, certain characteristic values (or limits of values) are to be expected for each degree of contractibility of interlayers. Actually, the characteristic charges of 10-Å unit structures and/or 16.8-Å unit structures in mixed-layer minerals and smectites have been determined by several authors (Table 1). Weaver and Pollard (1973) found the mean layer charge of montmorillonites and illites to be 0.81 and 1.44 esu/uc, respectively.

Assuming (1) the interaction of cation hydration energy and electrostatic force between the negative layer charge and the cation as the decisive factor for swelling properties of smectites and (2) a heterogenous distribution of layer charge for each kind of unit structure, the characteristic charges of the 10-, 14-, and 16.8-Å unit structures in monoionic potassium and ammonium smectites saturated with ethylene glycol were determined. The suitability of the method of "characteristic charges" for the determination of charge-density distribution was then ascertained.

### CALCULATIONS OF MEAN LOCAL CHARGE DENSITY OF LAYERS

#### *Formulation of the method*

The formation of an interstratified structure in each dioctahedral smectite was assumed to be influenced by

Table 1. Characteristic layer charge of 10-Å unit structure and 16.8-Å unit structure in mixed-layer minerals.

| Author(s)                    | Characteristic layer charge (esu/uc) |                     |
|------------------------------|--------------------------------------|---------------------|
|                              | 16.8-Å unit structure                | 10-Å unit structure |
| Hofmann <i>et al.</i> (1956) | 1.1                                  | 1.3                 |
| Brown and Weir (1963)        | 0.72                                 | 1.76                |
| Hower (1967)                 | <1.2                                 | >1.2                |
| Weaver (1968)                | 0.5–1.2                              | 1.2–2.0             |
| Besson <i>et al.</i> (1974)  |                                      | 1.2                 |
| Čičel and Machajdík (1978)   | 0.62 ± 0.24                          | 1.73 ± 0.14         |

the following factors: (1) The overall layer charge density and its distribution in the structure. (In the calculations tetrahedral and octahedral charges were not distinguished.) (2) The solvation energy of the cation. (3) The nature of the solvation agent.

For a given smectite the first factor is constant. By combinations of factors (2) and (3), various forms of interstratification of layers are possible. Cations with lower solvation energies and solvation agents with lower dipole moments bring about expansion of a smaller number of interlayers and vice versa. Electrostatic charge, formed by substitutions of cations in octahedral and tetrahedral sheets, attracts interlayer cations, and, thus, 10-Å layers tend to be formed. In such places in the structure, where the attraction forces prevail over the solvation forces, expansion is prevented regardless of the cation and solvation agent that are present in the interlayer. It is evident that the intensity of the attraction forces that would be necessary for the formation of 10-Å layers in the presence of a cation with low solvation energy will be smaller than in the presence of a cation with higher solvation energy. A similar consideration is valid also for solvation agents with various dipole moments ( $\mu$ ). Which of the three kinds of unit structures (10-, 14-, or 16.8-Å) is formed when a particular combination of interlayer cation and solvation agent is used, depends solely on the local charge density.

Characteristic negative charges QA, QC, and QE can be assigned which are necessary for formation of each layer. The sum of the proportion of each kind of layer multiplied by its respective charge must give the total charge of the layer.

$$(pA)(QA) + (pC)(QC) + (pE)(QE) = Q_t \quad (1)$$

where the probability coefficients pA, pC, and pE can be calculated from X-ray powder diffraction (XRD) data by the Fourier transform method. Total charge density,  $Q_t$ , can be calculated from the structural formula. (Symbols used in the present paper are the same as those used in Čičel and Machajdík (1981).) Thus, three unknowns are present in the equation, i.e.,

local charges of formation of the individual kinds of layers. Eq. (1) can be rewritten for three different samples:

$$\begin{aligned} (pA_1)(QA) + (pC_1)(QC) + (pE_1)(QE) &= Q_{t,1} \\ (pA_2)(QA) + (pC_2)(QC) + (pE_2)(QE) &= Q_{t,2} \quad (2) \\ (pA_3)(QA) + (pC_3)(QC) + (pE_3)(QE) &= Q_{t,3} \end{aligned}$$

If the probability coefficients and total charges of all three samples are known, the characteristic charges of the layers can be calculated. However, the exact values of the matrix of constants of the system are not known, and it is therefore necessary to describe the actual system of equations as follows

$$\begin{aligned} (pA_1 \pm \Delta pA_1)(QA) + (pC_1 \pm \Delta pC_1)(QC) \\ + (pE_1 \pm \Delta pE_1)(QE) &= Q_{t,1} \pm \Delta Q_{t,1} \\ (pA_1 \pm \Delta pA_2)(QA) + (pC_2 \pm \Delta pC_2)(QC) \\ + (pE_2 \pm \Delta pE_2)(QE) &= Q_{t,2} \pm \Delta Q_{t,2} \\ (pA_3 \pm \Delta pA_3)(QA) + (pC_3 \pm \Delta pC_3)(QC) \\ + (pE_3 \pm \Delta pE_3)(QE) &= Q_{t,3} \pm \Delta Q_{t,3} \end{aligned}$$

if charges QA, QC, and QE are equal in all of the studied samples, the values of the matrix of constants are responsible for errors in calculations. Hence, it follows that the correct values QA, QC, and QE can not be calculated if just one system of equations is used. This problem can be solved in two ways. First, it is possible to take a system of  $n$  equations (1), where  $n > 3$ , and then to use the least square method. Second, the  $n$  equations could be used to form a statistically significant number of systems of three equations with three unknowns, from which the average values of  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$  could be calculated. It is expected that the values of these charges will satisfy the relation

$$\overline{QA} > \overline{QC} > \overline{QE} > 0. \quad (4)$$

This relation can be used as one of the possible logical criteria for estimation of reliability of the calculated values. To obtain the average values of  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$ , both the least squares method, and the second method were used. The advantage of the second method is the fact that the individual deviations from average values of  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$  could be seen.

#### Calculations

For calculations of the characteristic charges, the analyzed interstratified structures and total charges calculated from the structural formulae reported by Čičel and Machajdík (1981) were used. The set of  $K^+$ -saturated and ethylene glycol-solvated smectites consisted of 12 samples. By writing Eq. (1) for each of them using the pertinent probability coefficients and  $Q_{tot}$  (Table 2), 12 equations with 3 unknowns QA, QC, and QE, were generated which were used to calculate the coefficients for the relation

$$Q_{tot} = f(pA, pC, pE). \quad (5)$$

Table 2. Selected probability coefficients of unit structures and layer charges for the samples reported by Čížek and Machajdík (1980).

| Sample number | Location <sup>1</sup>               | Q <sub>t</sub> | Probability coefficients for |      |      |                                |      |      |      |
|---------------|-------------------------------------|----------------|------------------------------|------|------|--------------------------------|------|------|------|
|               |                                     |                | K-smectite + EG              |      |      | NH <sub>4</sub> -smectite + EG |      |      |      |
|               |                                     |                | pA                           | pC   | pE   | pA                             | pC   | pE   | pAA  |
| 1             | Askangel, U.S.S.R.                  | 1.06           |                              | 0.36 | 0.64 | 0.07                           |      | 0.93 |      |
| 2             | Borša, Czechoslovakia               | 0.74           | 0.20                         |      | 0.80 | 0.12                           |      | 0.88 |      |
| 3             | Braňeny, Czechoslovakia             | 0.96           | 0.30                         | 0.10 | 0.60 | 0.16                           |      | 0.84 |      |
| 4             | Chambers, Arizona, U.S.A.           | 1.17           |                              | 0.75 | 0.25 | 0.06                           | 0.33 | 0.61 |      |
| 5             | Belle Fourche, South Dakota, U.S.A. | 0.86           | 0.14                         |      | 0.86 |                                |      | 1.00 |      |
| 6             | Jelšový Potok, Czechoslovakia       | 0.95           | 0.26                         | 0.12 | 0.62 | 0.09                           | 0.16 | 0.75 |      |
| 7             | Manito, Washington, U.S.A.          | 1.27           | 0.21                         | 0.69 | 0.10 | 0.14                           | 0.30 | 0.31 | 0.25 |
| 8             | Michajlov, Bulgaria                 | 1.16           | 0.35                         |      | 0.65 | 0.02                           |      | 0.98 |      |
| 9             | Polkville, Mississippi, U.S.A.      | 1.13           | 0.39                         | 0.18 | 0.43 | 0.09                           | 0.11 | 0.80 |      |
| 10            | Pyževskij, U.S.S.R.                 | 0.97           | 0.05                         | 0.17 | 0.78 |                                | 0.25 | 0.75 |      |
| 11            | Sampor, Czechoslovakia              | 1.12           | 0.15                         | 0.70 | 0.15 | 0.30                           |      | 0.70 |      |
| 12            | Zajsanskij, U.S.S.R.                | 0.63           |                              | 0.60 | 0.40 |                                | 0.05 | 0.83 | 0.12 |

Q<sub>t</sub> = total charge calculated for O<sub>20</sub>(OH)<sub>4</sub> (esu/unit cell); pA, pC, etc. = probability coefficients (pA for 10-Å, pC for 14-Å, pE for 16.8-Å, and pAA for 20-Å phase); EG = ethylene glycol saturated sample.

The general equation for the regression analysis is:

$$Q_{\text{tot}} = b_1 pA + b_2 pC + b_3 pE. \quad (6)$$

The numerical values of Eq. (6) were calculated by the method described by Ezekiel and Fox (1959) to give:

$$Q_{\text{tot}} = 2.05 pA + 1.29 pC + 0.33 pE. \quad (7)$$

The correlation coefficient is  $r = 0.96$  for this empirical relation. The coefficients in Eq. (7) represent the mean local layer charges:  $\overline{QA} = 2.05$  esu for 10-Å,  $\overline{QC} = 1.29$  esu for 14-Å, and  $\overline{QE} = 0.33$  esu for 16.8-Å thickness.

The second method yielded from the 12 empirical relations  $(12!/3!/12 - 3)! = 220$  systems of three equations with three unknowns. From these systems the mean local layer charges necessary for the formation of the unit structures  $A = 10$  Å,  $C = 14$  Å,  $E = 16.8$  Å can be calculated if the interlayer is saturated with K<sup>+</sup> and with ethylene glycol. A similar procedure was used to calculate those values for the set of samples saturated with NH<sub>4</sub><sup>+</sup> and solvated with ethylene glycol. For this calculation samples 7 and 12 were not used because the interpretation of the layer  $\overline{AA} = 20$  Å was questionable. The results are shown in Table 3.

The influence of errors inherent in the probability coefficients on the calculations of equation systems (QA, QC, and QE) was estimated by making control calculations, which showed that the system of Eq. (3) is very sensitive to the precision of input data and acts as an amplifier of errors which are entered into it in the form of incorrect values of the matrix of constants. The random scattering of individual values around the mean values of  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$  do not affect the mean values, as checked on two subsets of approximately 50 equation systems.

## DISCUSSION

The values  $\overline{QA}$ ,  $\overline{QC}$ , and  $\overline{QE}$  must be interpreted as average values. A unit structure A arises where the sum of local charges on two adjacent layers equals QA. It is probable that an interval exists around each characteristic charge within which the local charge may vary and the character of the unit structure remains unchanged. There are two reasons that justify this assumption: (1) It was assumed that there is no difference between the influence of the charge located on tetrahedral and octahedral sheets. In real structures with such a distribution of charges it can be expected that where the charge is localized on the inner tetrahedral sheet, a smaller charge will suffice for the formation of

Table 3. Average values of the characteristic charges on layers A, C, and E compared with charge and expandability of mica, vermiculite, and Ca-montmorillonite.

| Interlayer                                     | Local charge densities on the layer (esu/uc) |   |  |
|--|--|---|--|
|  | $\overline{QA}$                              | $\overline{QC}$                         | $\overline{QE}$                          |
| K <sup>+</sup> , ethylene glycol               | 1.99   | 1.20                                    | 0.56                                     |
| NH <sub>4</sub> <sup>+</sup> , ethylene glycol | 2.70   | 1.60                                    | 0.72                                     |
|  | Mica   | Vermiculite                             | Smectite                                 |
| Total layer charge (esu/uc)                    | 2  | 1-1.6                                   | 0.5-1.2                                  |
|  | no expansion                                 | complex with 1 layer of ethylene glycol | complex with 2 layers of ethylene glycol |

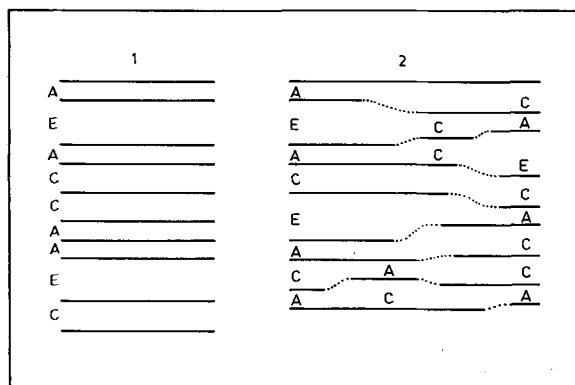


Figure 1. Schematic drawing of two possibilities of mixed layering.

the given kind of unit structure than would be necessary when charge is localized on the octahedral sheet or even when it is localized on the outer tetrahedral sheet. (2) Each interlayer space will acquire a state of solvation corresponding to one of the three interlayer distances (10, 14, and/or 16.8 Å) regardless of the effective charge density in it. Most probably it will be that interlayer whose mean local charge density is nearest to the effective charge density in the interlayer space of the two adjacent layers.

There is good agreement between the unit structures A, C, and E and their characteristic charges for  $K^+$ -treated samples with charges and expandability of mica, vermiculite (Bradley *et al.*, 1963), and smectites as they are shown in Table 3. This fact may be accepted as corroboration of the correctness of the calculated values. Larger values of these charges observed in  $NH_4^+$ -saturated samples can be explained by higher solvation energy of  $NH_4^+$  compared with that of  $K^+$ . This is why a greater charge is necessary to prevent an expansion of the interlayer. In spite of this, the QA seems to be too large. The occurrence of sites with such a high charge density is improbable in smectites. On the other hand, for  $NH_4^+$ -treated and ethylene glycol-solvated smectites the coefficient pA is very small (see Table 1), confirming that there are few such layers in the structure.

If the characteristic charges actually cause the formation of the individual unit structures in the interstratified structure, the probability coefficients may be reinterpreted. Because to each layer belongs a certain charge, the probability coefficients pA, pC, pE indicate the relative quantity of the respective charge in the structure. Thus, for example, sample 6 from Table 1 contains, according to the complex of  $K^+$ -saturated and ethylene glycol solvated samples, 26% layers with a charge of 1.99 esu/uc, 12% layers with a charge of 1.2

esu/uc, and 62% layers with a charge of 0.56 esu/uc. The  $NH_4^+$ -saturated and ethylene glycol solvated complex contains 9% layers with a charge 2.7 esu/uc, 16% layers with a charge of 1.6 esu/uc, and 75% layers with a charge of 0.72 esu/uc. Correctness of such an interpretation should be verified by another independent method for determination of charge density distribution, e.g., by the method proposed by Lagaly *et al.* (1976).

The description of an interstratified structure by probability coefficients does not say anything about the sequence of layers, i.e., whether the sequence of layers AC exists over the whole area of the layer A, or only in one part of it. The probability coefficients express the quantity of the individual layers and the quantity of the individual sequences. They do not express the way in which the layer sequences are arranged in the actual structure. Thus, it is not possible to make the decision whether a real structure resembles the type 1 or type 2 from Figure 1.

The attempt to calculate the characteristic charges QA, QB, and QD for smectite solvated with water molecules was unsuccessful because the samples were investigated at relative humidities which varied between 0.45 and 0.6. These samples contain the unit structures A = 10 Å, B = 12.6 Å, and D = 15.5 Å (Čížel and Machajdík, 1981). The same specimen studied at two different relative humidities contained various portions of expanded and non-expanded layers. In spite of this problem, the value of QA for the  $K^+$ -treated specimen, 1.3 esu/uc, and the value of QB, 0.86 esu/uc, were acceptable. No physical interpretation could be given for the charge QD or for all three charges of smectites saturated with  $NH_4^+$ .

## CONCLUSIONS

Analyses of 12 samples of monionic  $K^-$  and  $NH_4^+$ -smectites saturated by ethylene glycol allowed the calculation of the characteristic mean local charges necessary for the formation of 10-, 14-, and 16.8-Å unit structures. Values obtained for  $K^+$ -smectites (1.99, 1.20, and 0.56 esu/uc) corresponded fairly well with those of mica, vermiculite, and montmorillonite layer charges for which the above-mentioned unit structure distances are typical.

Significantly higher values of the characteristic mean charge density calculated for monoionic ammonium smectites saturated with ethylene glycol (2.7, 1.6, and 0.72 esu/uc) can be interpreted as a consequence of greater solvation energy of  $NH_4^+$  compared with that of  $K^+$ .

By the present method the characteristic mean charge density of layer formation for smectites treated with other monovalent cations (e.g.,  $Rb^+$ ,  $Cs^+$ ) can be calculated, as well as those treated with different solvation agents (water, glycerol, etc.).

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**Резюме**—Предполагается, что на образование внутринапластованной структуры в диоктаэдрическом смектите влияют: (1) полная плотность заряда слоя и её распределение в структуре. (2) энергия сольватации катиона, и (3) природа агента сольватации. Поддерживая факторы (2) и (3) постоянными, можно рассчитать средние плотности заряда QA, QC, и QE, необходимые для образования 10-, 14-, и 16,8-Å фаз со смешанными слоями в смектите, обработанном потасом и насыщенном этиленовым гликолем (ЭГ). Величины QA, QC, и QE, были 1,99, 1,2 и 0,56 э/эя (электростатическая единица/элементарная ячейка), соответственно. Для смектитов, обработанных аммонием, насыщенным ЭГ, соответствующие средние местные плотности заряда были 2,7, 1,6, и 0,72 э/эя. Были проведены расчеты при условии: QA > QC > QE > 0.

Для К-смектитов, насыщенным ЭГ,  $Q_{пол} = 1,99r_A + 1,2r_C + 0,56r_E$ , где:  $Q_{пол}$  = полный заряд;  $r_A$ ,  $r_C$ , и  $r_E$  = коэффициенты вероятности для 10-, 14-, и 16,8-Å фаз во внутринапластованной структуре. Вышеупомянутое уравнение, решенное при помощи метода наименьших квадратов и без ограничивающего условия, имеет вид:

$$Q_{пол} = 2,05r_A + 1,29r_C + 0,33r_E$$

Наблюдается хорошее соответствие между величинами слойного заряда для К-смектита и величинами для слюды, вермикулита и монтмориллонита, для которых вышеупомянутые расстояния элементарной структуры являются типичными. [Е.С.]



**Resümee**—Es wurde angenommen, daß die Bildung einer Wechsellagerungsstruktur in dioctaedischem Smektit beeinflußt wird durch (1) die gesamte Schichtladungsdichte und ihre Verteilung in der Struktur, (2) die Solvationsenergie des Kations, und (3) die Art des Lösungsmittels. Indem die Faktoren (2) und (3) konstant gehalten wurden, war es möglich die lokalen durchschnittlichen Ladungsdichten  $\overline{QA}$ ,  $\overline{QC}$  und  $\overline{QE}$  zu berechnen, die für die Bildung von 10-, 14- und 16.8-Å Wechsellagerungsphasen in Kalium-behandelten und Ethylenglycol (EG)-gesättigten Smektiten notwendig sind. Die werte von  $\overline{QA}$ ,  $\overline{QC}$ , und  $\overline{QE}$  betragen 1,99, 1,2 und 0,56 esu/uc, bzw. Ammonium-behandelte, EG-gesättigte Smektite gaben entsprechende mittlere lokale Ladungsdichten von 2,7, 1,6, und 0,72 esu/uc. Es wurden Berechnungen durchgeführt mit der Einschränkung  $QA > QC > QE > 0$ .

Bei EG-gesättigtem K-Smektit ergab sich  $Q_{tot} = 1,99pA + 1,2pC + 0,56pE$ , wobei  $Q_{tot}$  die Gesamtladung (esu/uc) ist, und pA, pC, und pE die Wahrscheinlichkeitskoeffizienten für die 10-, 14- und 16,8 Å-Phasen in der Wechsellagerungsstruktur darstellen. Die obere Gleichung, berechnet mit Hilfe der Methode der kleinsten Quadrate und ohne Nebenbedingung, ergibt

$$Q_{tot} = 2,05pA + 1,29pC + 0,33pE.$$

Es ergibt sich eine gute Übereinstimmung der Werte, die für K-Smektit-, Glimmer-, Vermiculit-, und Montmorillonitschichtladungen erhalten wurden, für die die oben erwähnten Einheitsstrukturabstände typisch sind. [U.W.]

**Résumé**—On a assumé que la formation d'une structure interstratifiée dans une smectite était influencée par (1) la densité de charge de couche totale, (2) l'énergie de solvation du cation, et (3) la nature de l'agent solvant. En gardant constants les facteurs (2) et (3), il était possible de calculer les densités de charge locales moyennes  $\overline{QA}$ ,  $\overline{QC}$ , et  $\overline{QE}$  qui sont nécessaires à la formation de phases mélangées 10-Å, 14-Å, et 16,8-Å dans les smectites traitées au potassium et saturées de glycol éthylène (EG). Les valeurs de  $\overline{QA}$ ,  $\overline{QC}$ , et  $\overline{QE}$  étaient respectivement 1,99, 1,2, et 0,56 esu/uc. Des smectites traitées à l'ammonium saturées de EG donnaient des densités de charge locales moyennes correspondantes de 2,7, 1,6, et 0,72 esu/uc. Les calculs ont été faits sous les conditions limitantes  $QA > QC > QE > 0$ .

Pour les smectites-K saturées de EG,  $Q_{tot} = 1,99pA + 1,2pC + 0,56pE$ , où  $Q_{tot}$  est la charge totale (esu/uc), et pA, pC, et pE sont des coefficients de probabilité pour les phases 10-Å, 14-Å, et 16,8-Å dans la structure interstratifiée. L'équation ci-dessus calculée à l'aide des carrés moindres et sous les conditions limitantes donne

$$Q_{tot} = 2,05pA + 1,29pC + 0,33pE$$

Les valeurs obtenues pour les smectites-K sont semblables à celles obtenues pour les charges de couche pour le mica, la vermiculite, et la montmorillonite pour lesquelles les distances de structure de maille ci-dessus sont typiques. [D.J.]