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# NOTES

## MINCALC1—A SPREADSHEET FOR THE RAPID CALCULATION OF 2:1 PHYLLOSILICATE MINERAL FORMULAE FROM CHEMICAL ANALYSES

**Key Words**—Clay mineral formulae, Spreadsheet.

The accurate calculation of clay mineral formulae from chemical analyses is important because the identity of the mineral as well as its exchange properties can be readily determined from its formula (Jackson 1969). Unfortunately, many mathematical steps, all fraught with possible errors, are required to carefully convert the data from either an oxide or metal basis to the structural formula. For one analysis, hand calculations are not that difficult to perform and, if done carefully, will yield the accurate formula. However, the time-effectiveness of hand calculations is severely dampened when determining more than one analysis. Because several analyses may be required to fully characterize the minerals in a sample, a spreadsheet program that can quickly and accurately determine the structural formulae for these analyses would be beneficial.

To this end, a spreadsheet program, named MINCALC1, that performs these structural formulae calculations for 2:1 phyllosilicates from the chemical data was developed. MINCALC1 has been tested using many chemical analyses and structural formulae calculations from the clay mineral literature. Because the spreadsheet was designed using charge occupancy rather than atom occupancy for the octahedral layer, the structural formulae of both dioctahedral and trioctahedral minerals can be quickly and accurately calculated.

### METHODOLOGY

The MINCALC1 spreadsheet was constructed using LOTUS 1-2-3® Release 3.1.[1] Release 3.1 was chosen because of its ability to handle and move between multiple worksheets in the same spreadsheet file. Other compatible formats include LOTUS 1-2-3® Release 4.0 as well as Borland's Quattro Pro® and Microsoft's Excel® data processing programs.

MINCALC1 is designed to calculate the structural formulae of 2:1 phyllosilicate minerals given the weight percentages of the following oxides: $SiO_2$, $TiO_2$, $Al_2O_3$, $Fe_2O_3$, FeO, MgO, CaO, $Na_2O$, and $K_2O$. Because the calculated formula is based on a $O_{10}(OH)_2$ format, the weight percentage of $H_2O$ is not inputed into the spreadsheet. The only other user input necessary is to choose whether Ti should be assigned to the tetrahedral or octahedral layer. Once these data inputs are completed, the spreadsheet instantly calculates the structural formula.

The underlying assumption in using this program is that the chemical data are strictly from a single 2:1 phyllosilicate mineral and do not include other particles that may be adhering to the surface of the mineral of interest. Excess silica, usually noticed as silica atoms greater than 4.0 in the tetrahedral layer of a half-unit cell formula, is typically associated with amorphous silica that was also present during the chemical analysis. Similarly, the quality of the chemical analysis can also be checked by examining the number of cations associated with the octahedral layers. Significant departures from the theoretical cation occupancy (2.0 for dioctahedral structures and 3.0 for trioctahedral structures) suggest the presence of more than one mineral during the chemical analysis.

As with any mineral formula calculation, a set of rules are necessary to prioritize the assignment of the cations to the structural positions (Jackson 1969). These same rules were followed for the MINCALC1 spreadsheet and are as follows: (1) the framework anionic charge is −22, (2) all Si is assigned to the tetrahedral layer to bring the total tetrahedral occupancy to 4 cations, (3) if a charge deficiency occurs in the tetrahedral layer following assignment of silicon, then Al and possibly $Fe^{3+}$ are assigned to the tetrahedral layer to bring the total tetrahedral cation occupancy to 4, (4) any remaining Al as well as Fe (either ferric or ferrous) are then assigned to the octahedral layer for a total octahedral charge of +6 (for handling both dioctahedral and trioctahedral structures), (5) any remaining charge deficit in the octahedral layer is balanced by the assignment of appropriate amounts of Mg to this layer, and (6) any remaining Mg as well as the other index cations (i.e., Ca, Na, K) are assigned to the interlayer

[1] The use of brand names in this report does not imply endorsement of these brands by the author.

Table 1. Chemical data of the examined minerals.

| Mineral name | $SiO_2$ | $Al_2O_3$ | $TiO_2$ | $Fe_2O_3$ | FeO | MgO | CaO | $K_2O$ | $Na_2O$ | $H_2O$ |
|---|---|---|---|---|---|---|---|---|---|---|
| | % | | | | | | | | | |
| Muscovite | 45.30 | 38.40 | | | | | | 11.80 | | 4.50 |
| Biotite | 41.30 | 11.80 | | | 9.90 | 22.10 | | 10.90 | | 4.10 |
| Talc | 63.50 | | | | | 31.70 | | | | 4.80 |
| Pyrophyllite | 66.70 | 28.30 | | | | | | | | 5.00 |
| Na-Montmorillonite† | 64.86 | 24.14 | 0.15 | 2.29 | | 3.39 | 0.61 | 0.10 | 3.94 | |
| Na-Saponite† | 58.44 | 5.04 | 0.03 | 1.90 | | 31.04 | 0.81 | 0.03 | 2.26 | |

† Data from Malla and Komarneni (1993).

positions. Charge balance is determined by independently assessing the contributions of the net layer charge from both the tetrahedral and octahedral layers and comparing this value to the charge associated with the interlayer cations.

The actual computational method for calculating the structural formula is the atomic/molecular proportions procedure of Hurlbut and Klein (1977). The atomic/molecular proportions of the cations and oxygens are normalized to 11 oxygens. Following proper assignment of the cations to the structural positions, the structural formula, charge balance information, and sum of tetrahedral and octahedral cations are then tabulated. This information can be used to quickly determine not only the identity of the mineral but also the character of the octahedral layer. Full details concerning the calculation and assignment of the cations are given in the brochure accompanying the program.

## EXAMPLES

The accuracy of the MINCALC1 spreadsheet can be observed by inputting the compositional data from an ideal formula and checking the calculated formula. For this exercise, the compositional data from the ideal formulae of muscovite [$KAl_2(Si_3Al)O_{10}(OH)_2$], biotite [$K(Mg_{0.8},Fe_{0.2})_3(Si_3Al)O_{10}(OH)_2$], pyrophyllite [$Al_2Si_4O_{10}(OH)_2$], and talc [$Mg_3Si_4O_{10}(OH)_2$] were used (Table 1). Comparisons between the ideal and MINCALC1 calculated formulae for these four minerals were, within rounding errors, identical (Table 2). These examples also illustrate the utility of the MINCALC1 spreadsheet for both dioctahedral and trioctahedral structures.

The results of the MINCALC1 spreadsheet have also been compared to many structural formulae given for smectites that have been published in the clay mineral literature, provided the compositional data were also published. As an example, Malla and Komarneni (1993) listed the results of the chemical analyses and the calculated structural formulae from both a Na-montmorillonite and Na-saponite (Tables 1 and 2). After entering their compositional data (which took <30 seconds), identical formulae, within rounding error, for these two minerals were calculated using MINCALC1 (Table 2). The speed and accuracy of the MINCALC1 spreadsheet therefore allows the researcher a rapid look as to the structural formula of the 2:1 phyllosilicate mineral being studied.

The real strength of MINCALC1 is not the calculation of accurate structural formulae, but that accurate formulae can be calculated very rapidly. MINCALC1 is no more accurate than hand calculations as both follow the same rules in their derivations of the structural formulae. However, MINCALC1 can provide the same formula as done by hand within seconds whereas 10–15 minutes are normally required for hand-derived structural formulae calculations.

In addition to research activities, this spreadsheet can also be used as a teaching tool. Several clay mineral compositions have been provided with the spreadsheet and may be quickly accessed using a macro. The structural formula is given and the student is asked, in mul-

Table 2. Comparison of the ideal and MINCALC1-derived structural formulae.

| Mineral name | Ideal mineral formula | Mineral formula using MINCALC1 |
|---|---|---|
| Muscovite | $KAl_2(Si_3Al)O_{10}(OH)_2$ | $KAl_2(Si_3Al)O_{10}(OH)_2$ |
| Biotite | $K(Mg_{2.40}Fe_{0.60})(Si_3Al)O_{10}(OH)_2$ | $K_{1.01}(Mg_{2.39}Fe_{0.60})(Si_3Al)O_{10}(OH)_2$ |
| Talc | $Mg_3Si_4O_{10}(OH)_2$ | $Mg_{2.98}Si_{4.01}O_{10}(OH)_2$ |
| Pyrophyllite | $Al_2Si_4O_{10}(OH)_2$ | $Al_2Si_4O_{10}(OH)_2$ |
| Na-Montmorillonite | $(K_{0.01}Na_{0.46}Ca_{0.04})(Mg_{0.30}Al_{1.57}Fe_{0.10})(Si_{3.87}Al_{0.13})O_{10}(OH)_2$† | $(K_{0.01}Na_{0.45}Ca_{0.04})(Mg_{0.30}Al_{1.56}Fe_{0.10})(Si_{3.86}Al_{0.13}Ti_{0.01})O_{10}(OH)_2$ |
| Na-Saponite | $(Na_{0.27}Ca_{0.05})(Mg_{2.87}Fe_{0.09})(Si_{3.63}Al_{0.37})O_{10}(OH)_2$† | $(Na_{0.27}Ca_{0.05})(Mg_{2.87}Fe_{0.09})(Si_{3.63}Al_{0.37})O_{10}(OH)_2$ |

† Structural formula taken from Malla and Komarneni (1993).

tiple choice format, the correct clay mineral name for the derived formula. The answer is quickly interpreted and given an appropriate message. Additional compositions can be easily input.[2]

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[2] Copies of MINCALC1 are available from the author by sending a blank diskette (either 5¼ or 3½ inch diskette) to him. Please state in your request which version of the program (developed using LOTUS 1-2-3®Release 3.1 or 4.0) you would like.