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SOFTWARE NOTICE

MINTAB: A general-purpose mineral recalculation and tabulation program for Macintosh microcomputers

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ABSTRACT

The program MINTAB calculates cation formula units from oxide weight percentages of mineral chemical analyses. Output is as conventional tables (columns = samples, rows = elements), as cations appended to the oxide input file (columns = elements, rows = samples), or both. Input ASCII files consist of tab-delimited analyses of up to 25 oxides in any order, prefaced by a label line that identifies the order. Minerals can be mixed in any order within the file, but are identified by a two-letter code (e.g., PX = pyroxene). Total Fe can be redistributed between Fe^{3+} and Fe^{2+} in appropriate minerals by using a generalized procedure (e.g., on the basis of 6 oxygens and 4 cations for pyroxene). This procedure can be applied globally to all appropriate mineral analyses or selectively to only those analyses that lack a value for Fe_2O_3. MINTAB can deal with traditional "wet" analyses (with values for H_2O, CO_2, P_2O_5, F, and/or Cl), as well as microprobe data.

INTRODUCTION—MINERAL RECALCULATION IN PRACTICE

The recalculation of mineral analyses into cationic formula units (usually to a fixed number of oxygens, e.g., O = 6 for pyroxenes) is a routine process in mineralogy and petrology. Programs to carry out such recalculations are implemented in most electron-microanalysis centers, and stand-alone general-purpose programs written for mainframe computers are also available (e.g., Freeborn et al., 1985), in addition to programs targeted at specific minerals (e.g., amphiboles, Rock, 1987; garnets, Knowles, 1987; micas, Rieder, 1977; pyroxenes, Ikeda, 1979). In our experience, many such programs are very useful, but they have disadvantages when it comes to tabulating and plotting data in reports and papers for many reasons, among which are the following: (1) Some programs are written in highly machine-specific source code (sometimes in obsolete dialects such as FORTRAN II or IV), which makes them difficult to implement on other computers. (2) Some programs deal only with a limited number of oxides and commonly cannot cope with minor but sometimes important elements such as V, Cr, Ni, Zn, Sr, Zr, Ba, or Pb, and especially F or Cl. (3) Some programs are designed for microprobe-style data and so cannot deal with analyses made by more traditional methods that may include values for oxides not capable of being analyzed by probe (e.g., Li_2O, H_2O, or CO_2 or separate values for both Fe_2O_3 and FeO). (4) Some programs can only cope with data output from the analytical equipment to which they are linked and do not allow processing of external data. (5) Output is rarely in the conventional tabular format preferred in publications (e.g., Table 1), and mixing of different mineral species as in Table 1 is commonly not allowed. (6) Output of the calculated cations to a machine-readable file may not be implemented, so that plots and further processing of the recalculated data cannot be performed without re-typing. (7) Procedures for reallocating total Fe (usually quoted in probe data as FeO) are not always implemented even for specific minerals where the process is relatively easy (e.g., pyroxenes) and are rarely implemented for all minerals that might be so treated. (8) Perhaps most important, several published programs have serious algorithmic problems: the garnet program by Knowles (1987), for example, gives invalid negative results for a large proportion of the garnet analyses in Deer et al. (1978), and we have obtained negative answers from the Fe reallocation procedures of some proprietary mineral-recalculation programs.

MINTAB grew out of a need to provide our own department with a mineral recalculation program that was user friendly, simple, and flexible but nevertheless free of all the above drawbacks. It has been extensively tested and verified with a large database of mineral analyses (including many data compiled by Deer et al. (1978), and the small subset used in Table 1).

SOFTWARE DESCRIPTION

MINTAB is based on an original FORTRAN program written for mainframe computers (PDP, DEC, VAX), which has now been rewritten in Think's Lightspeed Pascal and redesigned specifically for the increasingly popular Apple Macintosh range of microcomputers. It has been executed on all Macs from Plus to IIx and employs the exceptionally user-friendly Mac interface for maximum flexibility and accessibility. It has been tested under a wide range of system and machine configurations (up to System 6.0.2 under MULTIFINDER). Although the Mac is now extensively used in over 200 tertiary institutions throughout the world (particularly in North America), no mineral recalculation program for Macintosh computers has been published to our knowledge.

Input-file formats accepted

MINTAB accepts precisely the same type of input files as our other programs described recently in this journal (Wheatley and Rock, 1988; Rock and Carroll, 1989): namely, tab-delimited "text(only)" ASCII files (a universal Mac standard), in which

* Executable copies of MINTAB are available from the authors in exchange for other software. Please send disks with the software you are prepared to exchange. We will return your disks with a copy of MINTAB, a machine-readable copy of this documentation (or reprint), and a comprehensive test file of data that should give identical results to those in Deer et al. (1978). Users not able to exchange software are asked to send a nominal contribution (say US $10), in exchangeable form, to cover costs. We regret we are unable to deal with requests which only enclose a single disk. We ask users to refrain from copying MINTAB to third parties without reference to us and to cite this paper when MINTAB is used in their published work. Suggestions for improvements to MINTAB are welcomed.

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rows represent samples (analyses) and columns represent variables (oxides) and in which the first line must be a series of tab-delimited labels indicating the order of these variables (see below and Table 2 in Wheatley and Rock, 1988). Such files are readily generated, either directly by typing data into simple text editors such as EDIT or indirectly by typing data into spread-sheet or database applications such as STATVIEW, EXCEL, or 4TH DIMENSION and then saving the spread sheet as a "text (only)" file. For full instructions on this procedure, see the appropriate application manuals, including that for TRIPLOT (Rock and Carroll, 1989). Please note that MINTAB will not accept normal files produced by Mac applications such as MACWRITE or CRICKET GRAPH, since these use a program-specific binary format.

The present version of MINTAB is designed to handle up to 850 mineral analyses and 70 variables in one file. This capacity should be adequate to cope with most manageable research projects. MINTAB allows values "not analyzed" to be distinguished from those "analyzed but below detection limit" (Table 1): "not analyzed" (missing data) should be coded by the standard Mac "bullet" symbol (● = option 8), and will be ignored in all calculations, whereas "below detection limit" should be entered as some arbitrary real number (say, 0.00 or 0.01) and will be calculated as such. Simple error-trapping routines are also incorporated: for example, MINTAB will quit if it encounters any data values of <0 or >100 (neither of which should occur in percentage mineral analyses). Similarly, alphanumeric characters other than bullets are assumed to be erroneous, are converted to bullets, and hence are treated as missing values.

Input variables and values recognized

The following 25 variable names are specifically recognized by the present version of MINTAB, and assumed, if present, to head columns of real decimal numbers indicating percentages (e.g., 35.64): SiO2, Al2O3, Fe2O3, FeO, MgO, CaO, Na2O, K2O, H2O+, TiO2, P2O5, MnO, CO2, F, Cl, Li2O, V2O3 *or* V2O5, Cr2O3, NiO, ZnO, SrO, ZrO2, Nb2O5, BaO, PbO. These variables should cope with most significant mineral species. The first (label) line of the input file consists of a tab-delimited string of any combination of the above identifiers. This procedure enables oxide variables to be input in any order, for MINTAB will then rearrange them during processing. However, the identifiers must be specified *exactly as above*: for example, SiO2, not SIO2, sio2, Sio2, sIo2, Si or SI (subscripts cannot of course be used). Subsequent rows of actual data must of course conform to the order preset in the label line.

Any other variables (columns) identified as present by the label line of the input file, but not among the 25 specifically recognized above, will be treated as text strings, printed out "as is" in the output files and not reprocessed in any way. Thus the "H2O−," "H2O," and "DHZ-Total" rows in Table 1 are all ignored in the formula-unit calculations below. This option further allows sample labels or other identifiers to be input and output, using column headings other than the 25 variables specified above (e.g., "Sample," "Rock-type").

Minerals recognized

There is one further preset variable name, which can be used to tell MINTAB which minerals are present. If a column headed "Mineral" is present, it is assumed to contain one of a series of mineral-specifying codes (Table 2), from which the appropriate numbers of oxygens (and cations where appropriate) per formula unit are automatically preset. If MINTAB encounters an individual mineral that it does not recognize (i.e., its code is not in Table 2), a message is presented on screen to indicate that 10 oxygens will be used as the default for that analysis. If no "Mineral" column is present in the input file at all, MINTAB asks the user to provide a fixed number of oxygens to which all analyses in the input file are to be calculated.

Table 2 includes nearly all the significant rock-forming minerals but at present excludes phases whose precise formula units are variable or uncertain (e.g., idocrase, stilpnomelane), those whose chemistry is rarely determined (clay minerals, quartz), and those that require initial calculation to some fixed number of cations rather than oxygens (scapolite, sodalite group). Hence, files consisting entirely of one of these excluded minerals should not include a "Mineral" column at all but assign the number of oxygens at execution time. On the other hand, users with one or two excluded mineral analyses among a set of minerals otherwise covered by Table 2 should include a "Mineral" column (to cater to most of the data) with the rare mineral annotated as XX (Table 2) and should then recalculate that particular analysis to some other formula-unit convention retrospectively.

Treatment of H_2O, F, and Cl

If MINTAB encounters an H_2O+ value for any individual analysis, it proceeds as follows: (1) If the mineral is a recognized rock-forming mineral with essential water (amphibole, analcime, chlorite, etc.), the preset number of oxygens is adjusted upward so as to calculate on the basis of [O,OH] instead of [O] alone (as in Table 2; see Table 1, no. 2). (2) For any other recognized rock-forming mineral in Table 2, the H_2O value is treated as an impurity and set to zero in the formula unit, following Deer et al. (1978). Note that only values labeled "H2O+" are considered; "H2O−," "H2O," "LOI," etc. are always ignored.

It could be argued that many other constituents (e.g., K_2O in pyroxenes, Na_2O in garnets) should also be treated as impurities, but there may also be circumstances in which such constituents are critical (e.g., K_2O is now widely recognized as being a real and genetically significant component in high-pressure pyroxenes from kimberlites). It was therefore preferable to leave users with the option (and responsibility) of refraining from inputting constituents that they consider inaccurate or foreign. Except for H_2O in the nominally anhydrous rock-forming minerals in Table 2, therefore, all oxides will be treated by MINTAB as real.

Recalculation of microprobe data for minerals with F and Cl as well as H_2O+ presents a problem for any mineral-recalculation program. It is conventional, for example, to calculate amphiboles to 24[O,OH,F,Cl] where H_2O+ is determined but to 23[O] where it is not. However, a typical microprobe analysis with F or Cl but no H_2O+ ideally needs to be calculated to a variable oxygen equivalent, depending on how much F or Cl is actually present: that is, to 23[O] where [F + Cl] is near-zero and to 24[F,Cl] where [F + Cl] approaches 2.0 (in fluoramphiboles or chloramphiboles). Unfortunately, this requires the answer to be known before the question is put, and is thus difficult to program simply. Since the difference amounts to only about 4% even for microprobe analyses of the very rare fluor- or chloramphiboles, micas or sphenes, MINTAB retains the normal convention of calculating to 23[O] without H_2O+, and to 24[O] with H_2O+ determined.

Additional options

In operation, MINTAB presents three Mac dialog boxes that select a series of other options: (1) If P_2O_5 and CO_2 are detected in the input file, MINTAB asks whether these two oxides are to be removed as apatite and calcite, respectively, or ignored. This procedure allows for impurities in some wet chemical analyses. The same dialog also allows for unidentified minerals, as just

Table 1. MINTAB output as conventional tables (columns = samples, rows = variables)*

(a) With global Fe reallocation†

	1	2	3	4	5	6	7	8	9	10
#Mineral	FP	BI	PX	PX	GT	GT	IL	IL	SP	SP
SiO2	65.76	38.22	57.73	51.92	38.03	36.10	•	0.51	0.12	•
TiO2	0.08	2.96	0.04	0.77	•	1.21	52.73	50.02	•	0.13
Al2O3	20.23	14.71	0.95	1.85	22.05	20.90	•	•	55.97	65.40
Fe2O3	0.18	3.83	0.42	31.44	0.88	•	•	4.19	•	4.32
FeO	•	13.44	3.57	0.75	29.17	36.80	45.83	42.18	7.90	8.03
MgO	0.10	13.45	36.13	•	6.49	1.33	1.25	0.46	0.12	22.23
BaO	0.63	•	•	•	•	•	•	•	•	•
CaO	1.19	1.46	0.23	•	1.80	0.57	•	0.71	0.01	•
Na2O	8.44	0.50	•	12.86	•	•	•	•	•	•
K2O	3.29	7.90	•	0.19	•	•	•	•	•	•
H2O+	0.37	1.89	0.52	0.17	0.48	•	•	•	•	•
H2O-	0.08	0.60	0.04	•	0.16	•	•	•	•	•
H2O	•	•	•	•	•	•	•	0.13	•	•
Cr2O3	•	•	0.46	•	•	•	•	•	•	•
NiO	•	•	0.35	•	•	•	•	•	•	•
MnO	•	0.52	0.08	•	1.57	2.50	•	1.44	0.42	0.10
ZnO	•	•	•	•	•	•	•	•	35.85	0.24
DHZ-Total	100.35	•	100.52	•	99.99	•	•	99.64	100.32	100.45
‡CalcTotal	99.90	98.88	99.92	96.64	99.90	99.41	99.81	99.09	100.39	100.02
OxNum	8	24	6	6	12	12	3	3	32	32
Si	2.930	5.867	1.974	1.994	2.982	2.958	0.000	0.013	0.029	0.000
Al	1.062	2.661	0.038	0.084	2.038	2.018	0.000	0.000	15.878	15.346
Fe3	0.006	0.442	•	0.851	•	•	0.013	0.075	0.064	0.615
Fe2	0.000	1.725	0.113	0.082	1.965	2.522	0.947	0.895	1.526	1.369
Mg	0.007	3.078	1.841	0.000	0.759	0.162	0.047	0.017	0.043	6.598
Ca	0.057	0.240	0.008	0.000	0.151	0.050	0.000	0.019	0.003	0.000
Na	0.729	0.149	0.000	0.958	0.000	0.000	0.000	0.000	0.000	0.000
K	0.187	1.547	0.000	0.009	0.000	0.000	0.000	0.000	0.000	0.000
H	0.000	1.935	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ti	0.003	0.342	0.001	0.022	0.000	0.075	0.993	0.950	0.000	0.019
Mn	0.000	0.068	0.002	0.000	0.104	0.174	0.000	0.031	0.086	0.017
Cr	0.000	0.000	0.012	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ni	0.000	0.000	0.010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Zn	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6.371	0.035
Ba	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
◊mg	1.000	0.641	0.942	0.000	0.279	0.060	0.047	0.019	0.027	0.828
Total Cat	4.991	18.055	3.999	4.000	6.999	6.958	2.000	2.000	24.000	24.000
Ox Equiv	8.000	24.000	6.000	6.000	12.000	12.000	3.000	3.000	32.000	32.000
§New Fe2O3	•	•	•	29.427	•	•	0.714	3.946	0.353	4.105
§New FeO	•	•	•	2.566	•	•	45.187	42.400	7.582	8.224
¶New Calc Total	•	•	•	99.58	•	•	99.88	99.49	100.43	100.43
ΔReallo Code	1	1	3	2	3	3	2	2	2	2
Albite	74.940	•	•	•	•	•	•	•	•	•
Anorthite	5.839	•	•	•	•	•	•	•	•	•
Orthoclase	19.221	•	•	•	•	•	•	•	•	•
Enstatite	•	•	99.871	0.000	•	•	•	•	•	•
Ferrosilite	•	•	0.120	100.000	•	•	•	•	•	•
Wollastonite	•	•	0.009	0.000	•	•	•	•	•	•

(b) With selective Fe reallocation†

	1	2	3	4	5	6	7	8	9	10
#Mineral	FP	BI	PX	PX	GT	GT	IL	IL	SP	SP
SiO2	65.76	38.22	57.73	51.92	38.03	36.10	•	0.51	0.12	•
TiO2	0.08	2.96	0.04	0.77	•	1.21	52.73	50.02	•	0.13
Al2O3	20.23	14.71	0.95	1.85	22.05	20.90	•	•	55.97	65.40
Fe2O3	0.18	3.83	0.42	31.44	0.88	•	•	4.19	•	4.32
FeO	•	13.44	3.57	0.75	29.17	36.80	45.83	42.18	7.90	8.03
MgO	0.10	13.45	36.13	•	6.49	1.33	1.25	0.46	0.12	22.23
BaO	0.63	•	•	•	•	•	•	•	•	•
CaO	1.19	1.46	0.23	•	1.80	0.57	•	0.71	0.01	•
Na2O	8.44	0.50	•	12.86	•	•	•	•	•	•
K2O	3.29	7.90	•	0.19	•	•	•	•	•	•
H2O+	0.37	1.89	0.52	0.17	0.48	•	•	•	•	•
H2O-	0.08	0.60	0.04	•	0.16	•	•	•	•	•
H2O	•	•	•	•	•	•	•	0.13	•	•
Cr2O3	•	•	0.46	•	•	•	•	•	•	•
NiO	•	•	0.35	•	•	•	•	•	•	•
MnO	•	0.52	0.08	•	1.57	2.50	•	1.44	0.42	0.10
ZnO	•	•	•	•	•	•	•	•	35.85	0.24
DHZ-Total	100.35	•	100.52	•	99.99	•	•	99.64	100.32	100.45
‡CalcTotal	99.90	98.88	99.96	99.78	99.99	99.41	99.81	99.51	100.39	100.45
OxNum	8	24	6	6	12	12	3	3	32	32
Si	2.930	5.867	1.972	1.985	2.976	2.958	0.000	0.013	0.029	0.000
Al	1.062	2.661	0.038	0.083	2.033	2.018	0.000	0.000	15.878	15.338
Fe3	0.006	0.442	0.011	0.904	0.052	•	0.013	0.080	0.064	0.647
Fe2	0.000	1.725	0.102	0.024	1.909	2.522	0.947	0.890	1.526	1.336
Mg	0.007	3.078	1.840	0.000	0.757	0.162	0.047	0.017	0.043	6.595
Ca	0.057	0.240	0.008	0.000	0.151	0.050	0.000	0.019	0.003	0.000
Na	0.729	0.149	0.000	0.953	0.000	0.000	0.000	0.000	0.000	0.000
K	0.187	1.547	0.000	0.009	0.000	0.000	0.000	0.000	0.000	0.000
H	0.000	1.935	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ti	0.003	0.342	0.001	0.022	0.000	0.075	0.993	0.949	0.000	0.019
Mn	0.000	0.068	0.002	0.000	0.104	0.174	0.000	0.031	0.086	0.017
Cr	0.000	0.000	0.012	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ni	0.000	0.000	0.010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Zn	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6.371	0.035
Ba	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
◊mg	1.000	0.641	0.947	0.000	0.284	0.060	0.047	0.019	0.027	0.831
Total Cat	4.991	18.055	3.996	3.981	7.982	6.958	2.000	1.998	24.000	23.988
Ox Equiv	8.000	24.000	6.000	6.000	12.000	12.000	3.000	3.000	32.000	32.000
§New Fe2O3	•	•	•	•	•	•	0.714	•	0.353	•
§New FeO	•	•	•	•	•	•	45.187	•	7.582	•
¶New Calc Total	•	•	•	•	•	•	99.88	•	100.43	•
ΔReallo Code	1	1	1	1	1	3	2	1	2	1
Albite	74.940	•	•	•	•	•	•	•	•	•
Anorthite	5.839	•	•	•	•	•	•	•	•	•
Orthoclase	19.221	•	•	•	•	•	•	•	•	•
Enstatite	•	•	99.884	0.000	•	•	•	•	•	•
Ferrosilite	•	•	0.108	100.000	•	•	•	•	•	•
Wollastonite	•	•	0.009	0.000	•	•	•	•	•	•

*MINTAB generates these as ASCII text(only) files, which can be read directly by most Macintosh applications; top half of both tables (down to 'DHZ-total') is input data, bottom half is parameters output by MINTAB

†See text for explanation

#All analyses from Deer et al.(1962,1978)

‡Calculated total of input oxides (adjusted for O=Cl, O=F)

§Wt.% Fe oxides after reallocation (where carried out)

¶Oxide total adjusted for Fe reallocation (where carried out)

◊ mg = molecular $Mg/[Mg+Fe^{2+}]$

ΔResult of Fe reallocation procedure, codified as follows: 1 = inappropriate mineral (Table 2), or reallocation suppressed

2 = reallocation successful (cation and oxygen totals in Table 2 both achieved)

3 = reallocation impossible (e.g. total cations lower than ideal total in Table 2, with all Fe as FeO)

4 = reallocation only partially successful (e.g. all Fe as FeO has been converted to Fe_2O_3 but cation total remains below ideal value in Table 2)

TABLE 2. Mineral codes recognized in MINTAB and conventions for formula-unit recalculation

Mineral	Code	Oxygens*	Fe reallocation procedure (Droop, 1987)
Al_2SiO_5	AS	20	Not necessary
Amphiboles	AM	23 or 24†	To be implemented‡
Analcimes	AC	6 or 7†	Not necessary
Biotites	BI	22 or 24†	Not applicable
Carbonates	CB	4§	Not necessary
Chlorites	CH	28 or 36†	Not applicable
Chloritoids	CI	12 or 14†	Not applicable
Cordierites	CD	18	Not necessary
Epidotes	EP	25 or 13†	Not applicable
Feldspars	FP	8	Not necessary
Garnets	GT	12	→12 oxygens, 8 cations
Ilmenites	IL	3	→3 oxygens, 2 cations
Kalsilites	use NE	32	Not necessary
Leucites	LC	6	Not necessary
Melilites	ME	14	Not necessary
Monticellites	use OL	4	Not necessary
Muscovites	use BI	22 or 24†	Not applicable
Nephelines	NE	32	Not necessary
Olivines	OL	4	Not necessary
Perovskites	PV	3	Not necessary
Petalite	use XX	10	Not necessary
Pyrophyllite	use BI	22 or 24†	Not applicable
Pyroxenes and pyroxenoids	PX	6	→6 oxygens, 4 cations
Sapphirines	SA	20	→20 oxygens, 14 cations
Serpentines	use CH	28 or 36†	Not applicable
Sphenes	SE	20	Not necessary
Spinels	SP	32	→32 oxygens, 24 cations
Staurolites	ST	46 or 48†	Not applicable
Talc	use BI	22 or 24†	Not applicable
Wollastonite	use PX	6	→6 oxygens, 4 cations
Zircon	ZC	16	Not necessary
Unspecified	XX	10	—

* Number of oxygens follows conventions in Deer et al. (1978).
† First value is used if $H_2O = 0$ or missing, second if $H_2O > 0$; this procedure does not cover Cl- or F-rich compositions.
‡ There is no agreed-upon procedure for amphiboles; the IMA (1978) report is currently being revised by the IMA amphibole subcommittee, and possible procedures are being considered; if one is recommended or imposed, it will be added to MINTAB in due course.
§ Assumes CO_2 not determined.

mentioned. (2) MINTAB questions how Fe is to be reallocated, as described in the next section. (3) MINTAB inquires whether the calculated cations are to be appended to the input file (thus generating output like Fig. 1), or whether a new output file is to be generated in conventional tabular format (columns = analyses, rows = oxides and cations, thus generating output like Table 1), or both. In any case, output files are in the same electronic form as input: namely, tab-delimited, "text (only)" (ASCII) files, which can be quickly and readily imported into most other Macintosh applications for subsequent word processing, plotting, or subsidiary data analysis (as in Fig. 1).

Output formats

In both tabulated and appended output formats, oxides (top half of Table 1; first 19 columns of Fig. 1) are listed in the same order for output as for input, including any which are not used in the formula-unit recalculations. However, cations are output in the order Si, Al, Fe^3, Fe^2, Mg, Ca, Na, K, H, Ti, Mn, F, Cl, V, Cr, Ni, Zn, Sr, Zr, Nb, Ba, Pb (i.e., major cations in the order adopted by the U.S. and British Geological Surveys, minor cations in order of atomic number). Certain other calculations are made in addition, as annotated in Table 1.

MINERAL NAMES AND END-MEMBERS

MINTAB automatically calculates simple ternary end-members for feldspars and pyroxenes, and olivine end-members are of course given by molecular $Mg/(Mg + Fe^{2+})$ ratios, which are calculated in all cases (cf. Table 1). However, it does not at present name all possible output mineral components in full, largely because there is no IMA-accepted nomenclature for most mineral groups. Furthermore, implementation of the existing IMA schemes is not timely: the amphibole-nomenclature scheme (Leake, 1978) is currently undergoing revision, and the recent pyroxene-nomenclature scheme (Morimoto, 1988) has many ambiguities (Rock, in preparation). It is hoped, nevertheless, to add naming of the more complex species to MINTAB in due course.

Calculation of mineral norms (i.e., the proportions of large sets of end-members in, for example, pyroxenes and garnets) is also beyond the scope of MINTAB as implemented at present, mainly because there is no standard way of calculating end-members and because the necessary procedures for all the minerals accommodated by MINTAB would make the program unacceptably bulky.

REALLOCATION OF TOTAL Fe

The reallocation of microprobe-determined Fe between Fe^{3+} and Fe^{2+} can be carried out on the basis of various structural, stoichiometric, or charge-balance considerations (e.g., Finger, 1972; Cawthorn and Collerson, 1974; Papike et al., 1974; Lucas et al., 1989). MINTAB implements the general procedure of Droop (1987), which applies to most common minerals in which either the sum, or the sum of some subset of the cations, can be considered to be fixed for a fixed number of oxygens: for example, pyroxenes (4 total cations per 6 oxygens), and garnets (8 cations

	Mineral	SiO2	TiO2	Al2O3	Fe2O3	FeO	MgO	BaO	CaO	Na2O	K2O	H2O+	H2O-	H2O	Cr2O3
1	FP	65.76	.08	20.23	.18	•	.10	.63	1.19	8.44	3.29	.37	.08	•	•
2	BI	38.22	2.96	14.71	3.83	13.44	13.45	•	1.46	.50	7.90	1.89	.60	•	•
3	PX	57.73	.04	.95	.42	3.57	36.13	•	.23	•	•	.52	.04	•	.46
4	PX	51.92	.77	1.85	31.44	.75	•	•	•	12.86	.19	.17	•	•	•
5	GT	38.03	•	22.05	.88	29.17	6.49	•	1.80	•	•	.48	.16	•	•
6	GT	36.10	1.21	20.90	•	36.80	1.33	•	.57	•	•	•	•	•	•
7	IL	•	52.73	•	•	45.83	1.25	•	•	•	•	•	•	•	•
8	IL	.51	50.02	•	4.19	42.18	.46	•	.71	•	•	•	•	.13	•
9	SP	.12	•	55.97	•	7.90	.12	•	.01	•	•	•	•	•	•
10	SP	•	.13	65.40	4.32	8.03	22.23	•	•	•	•	•	•	•	•

	NiO	MnO	ZnO	DHZ-Total	CalcTotal	OxNum	Si	Al	Fe3	Fe2	Mg	Ca	Na	K
1	•	•	•	100.35	99.90	8	2.930	1.062	.006	0	.007	.057	.729	.187
2	•	.52	•	•	98.88	24	5.867	2.661	.442	1.725	3.078	.240	.149	1.547
3	.35	.08	•	100.52	99.92	6	1.974	.038	•	.113	1.841	.008	0	0
4	•	•	•	•	96.64	6	1.994	.084	.851	.082	0	0	.958	.009
5	•	1.57	•	99.99	99.90	12	2.982	2.038	•	1.965	.759	.151	0	0
6	•	2.50	•	•	99.41	12	2.958	2.018	•	2.522	.162	.050	0	0
7	•	•	•	•	99.81	3	0	0	.013	.947	.047	0	0	0
8	•	1.44	•	99.64	99.09	3	.013	0	.075	.895	.017	.019	0	0
9	•	.42	35.85	100.32	100.39	32	.029	15.878	.064	1.526	.043	.003	0	0
10	•	.10	.24	100.45	100.02	32	0	15.346	.615	1.369	6.598	0	0	0

	H	Ti	Mn	Cr	Ni	Zn	Ba	Total Cat	Ox Equiv	New Fe2O3	New FeO	New Calc Total
1	0	.003	0	0	0	0	.011	4.991	8	•	•	•
2	1.935	.342	.068	0	0	0	0	18.055	24	•	•	•
3	0	.001	.002	.012	.010	0	0	3.000	6	•	•	•
4	0	.022	0	0	0	0	0	4.000	6	29.43	2.566	99.58
5	0	0	.104	0	0	0	0	6.999	12	•	•	•
6	0	.075	.174	0	0	0	0	6.958	12	•	•	•
7	0	.993	0	0	0	0	0	2.000	3	.71	45.187	99.88
8	0	.950	.031	0	0	0	0	2.000	3	3.95	42.400	99.49
9	0	0	.086	0	0	6.371	0	24.000	32	.35	7.582	100.43
10	0	.019	.017	0	0	.035	0	24.000	32	4.11	8.224	100.43

	Reallo Code	Albite	Anorthite	Orthoclase	Enstatite	Ferrosilite	Wollastonite
1	1	2.9	5.867	1.974	1.994	2.982	2.958
2	1	1.1	2.661	.038	.084	2.038	2.018
3	3	6.0E-3	.442	•	.851	•	•
4	2	0	1.725	.113	.082	1.965	2.522
5	3	7.0E-3	3.078	1.841	0	.759	.162
6	3	.1	.240	.008	0	.151	.050
7	2	.7	.149	0	.958	0	0
8	2	.2	1.547	0	.009	0	0
9	2	0	1.935	0	0	0	0
10	2	3.0E-3	.342	.001	.022	0	.075

Fig. 1. MINTAB output with results appended to input file (columns = variables, rows = samples). The actual MINTAB text(only) output file has subsequently been imported directly into STATVIEW II for printing, and corresponds exactly to the results in Table 1a. Import into STATVIEW allows further sophisticated graphical and statistical processing, such as *X-Y* plots, histograms, formulae, transformations, etc. Note that STATVIEW has split up the file during printing into four segments, but the actual file consists of one continuous 48 column × 10 row spread sheet.

per 12 oxygens). Droop's procedure is a generalization of several that have been suggested in the literature for specific minerals, and it produces exactly the same answers as most of these procedures.

Minerals for which no such recalculation is possible include those with no fixed cationic number (e.g., micas), those with $Si^{4+} = 4H^+$ substitution (e.g., staurolite), those with essential amounts of nonanalyzed elements (e.g., boron-bearing minerals), those with nonessential quantities of Fe (e.g., feldspars), and those in which Fe is almost entirely as FeO (e.g., olivines) or Fe_2O_3 (e.g., epidotes). Formulae of all these minerals are calculated exactly from the Fe_2O_3 or FeO values provided in the input file (Table 1, nos. 1–2).

Droop's procedure also assumes that there is only one element with more than one oxidation state (i.e., Fe); calculation of, for example, Ti^{3+} and Mn^{3+} in pyroxenes requires a substantially more complex and specialized procedure and is being implemented as a separate program (Rock, in preparation).

The user has three additional options for regulating the extent to which Fe is reallocated: (1) No reallocation—reallocation is suppressed even if appropriate minerals are present. (2) Global reallocation (Table 1a)—all analyses of appropriate minerals in Table 2 (pyroxene, etc.) are reallocated, irrespective of whether each analysis contains values for both Fe oxides or for only one Fe oxide. (3) Selective reallocation (Table 1b)—an analysis of an appropriate mineral is reallocated if a value for FeO only is provided, but if values for both Fe_2O_3 and FeO are given, the analysis is not reallocated (this option allows MINTAB to treat cases where Fe has been carefully analyzed by, say, wet or Mössbauer methods, so that separate Fe_2O_3 and FeO are known with confidence).

Thus, Fe in analyses 4, 8, and 10 has been reallocated in Table 1a but not in Table 1b, because each analysis contains values for both Fe_2O_3 and FeO, whereas the Fe in analyses 7 and 9 has been reallocated in both tables. With each of these options, a code (1, 2, 3, or 4) is added to the output file to indicate the success or failure of the procedure (Table 1). For example, reallocation was successful with Table 1a, nos. 4 and 7–10, but it failed with nos. 3, 5, and 6 because total cations are too low with total Fe given as FeO (conditions $S < T$ in the nomenclature of Droop, 1987).

Using a database of hundreds of spinel and ilmenite analyses of maximum variability, we have checked the Droop (1987) Fe reallocation procedure used in MINTAB against two other procedures commonly used: that of Finger (1972) and a procedure for spinels in which, after calculating to 32 oxygens, Fe^{3+} is calculated as $[16 - (Al + Cr + 2Ti + V)]$ and Fe^{2+} = total Fe − Fe^{3+} with the calculation for Fe^{3+} and O repeated until the mineral formula converges. Differences between MINTAB and the other procedures are minimal for all but a tiny minority of extremely rare compositions. They are less than differences that can arise from analytical error or, legitimately, from varying treatment of, say, Si impurities. The correlation between MINTAB Fe^{3+} and the other methods is >0.99, and the regression line closely approximates $Y = X$. The results agree even for ilmenites with as much as 47% Fe_2O_3 and spinels with almost 12% Fe_2O_3. Plots of the results can be supplied on request.

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References cited

Cawthorn, R.G., and Collerson, K.D. (1974) The recalculation of pyroxene end-member parameters and the estimation of ferrous and ferric iron content from electron microprobe analyses. American Mineralogist, 64, 102–108.

Deer, W.A., Howie, R.A., and Zussman, J. (1978) Rock-forming minerals (2nd edition). Longmans, London.

Droop, G.T.R. (1987) A general equation for estimating Fe^{3+} concentrations in ferromagnesian silicates and oxides from microprobe analyses, using stoichiometric criteria. Mineralogical Magazine, 51, 431–435.

Finger, L.W. (1972) The uncertainty of the calculated ferric iron content of a microprobe analysis. Carnegie Institution of Washington Year Book 71, 600–603.

Freeborn, W.P., McGee, E.S., and Huebner, J.S. (1985) MINCLC: A FORTRAN program for recalculating mineral analyses. U.S. Geological Survey Open-File Report, 85–257.

Ikeda, K. (1979) Calculation procedure of end-members of clinopyroxenes, computer program and estimation of ferric and ferrous in EPMA analyses. Journal of the Japanese Association of Mineralogists and Economic Geologists, 74, 135–149.

Knowles, C.R. (1987) A BASIC program to recast garnet end-members. Computers and Geosciences, 13, 655–659.

Leake, B.E. (1978) Nomenclature of amphiboles. American Mineralogist, 63, 1023–1052.

Lucas, H., Muggeridge, M.T., and McConchie, D.M. (1989) Iron in kimberlitic ilmenites and chromian spinels: A survey of analytical techniques. Special Publication, Geological Society of Australia, 14, 311–320.

Morimoto, N. (1988) Nomenclature of pyroxenes. American Mineralogist, 73, 1123–1133.

Papike, J.J., Cameron, K.L., and Baldwin, K. (1974) Amphiboles and pyroxenes: Characterization of other than quadrilateral components and estimates of ferric iron from microprobe data. Geological Society of America Abstracts with Programs, 6, 1035.

Rieder, M. (1977) Micas: Recalculation of crystallochemical formulae by a FORTRAN IV program. Vestnik Ustredního ústava geologického, 52, 333–342.

Rock, N.M.S. (1987) A FORTRAN program for tabulating and naming amphibole analyses according to the International Mineralogical Association scheme. Mineralogy and Petrology, 37, 79–88.

Rock, N.M.S., and Carroll, G.W. (1989) TRIPLOT and ACF: General-purpose and metamorphic ACF-AKF-AFM triangular plotting programs for mainframes and microcomputers. American Mineralogist, 74, 277–280.

Wheatley, M.R., and Rock, N.M.S. (1988) SPIDER: A Macintosh program to generate normalized multi-element "spidergrams." American Mineralogist, 73, 919–921.

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