# SOFTWARE NOTICE

## RECALC2—A package for processing mineral analyses produced by electron microprobe

BRENDON J. GRIFFIN, JANET R. MUHLING   Electron Microscopy Centre, University of Western Australia, Nedlands, Western Australia 6009, Australia

GARY W. CARROLL, NICHOLAS M. S. ROCK   Key Centre for Teaching and Research in Strategic Mineral Deposits, Department of Geology, University of Western Australia, Nedlands, Western Australia 6009, Australia

### INTRODUCTION

RECALC2 is a package of programs designed to simplify the assessment and manipulation of mineral analyses produced by electron microprobe. It is designed to assist inexperienced users who commonly do not have a good grasp of mineral chemistry, but also provides data in a form usable by experienced analysts. It differs from the MINFILE package (Afifi and Essene, 1988) in that a complete output listing is produced that allows assessment of analysis quality and does not require sorting of analyses by mineral group before processing.

Processing of mineral analyses produced by electron microprobes can be a lengthy and hazardous process if performed by hand. The steps involved can be summarized as:

Part I: Acquisition and recalculation of data

1. collection of data from the microprobe;
2. estimation of $Fe_2O_3$ contents for ferromagnesian silicates and oxides where applicable;
3. conversion of wt% oxide to wt% carbonate for carbonate analyses;
4. calculation of numbers of cations per formula unit for each analysis;
5. calculation of end-member proportions where appropriate;
6. assessment of analysis quality from stoichiometry, charge balance, and analysis total;

Part II: Manipulation of data

7. sorting of analyses by mineral type or sample group;
8. preparation and printing of tables;
9. preparation and plotting of figures.

The RECALC2 package is designed to perform Part I of this task automatically, with the minimum of knowledge and input from the analyst. The objectives of the package are (1) Ease of use. For steps 1–6 all that is required is the input of mineral types and filenames as prompted. (2) Easy assessment of analysis quality so that inferior analyses can be recognized and discarded. To this end, a full output is produced that lists site occupancies and other relevant data. (3) Ease of preparation of tables and figures for publication. The full output produced as in (2) above is unsuitable for publication. Commercially available spreadsheet packages are probably the best environment for manipulating data, and therefore additional output files are produced that can be read into such packages.

### DESCRIPTION

The RECALC2 package comprises 16 programs written in Microsoft QuickBASIC and will run on 640 kilobyte RAM or bigger IBM XT and AT compatible PCs. The package comprises (1) the RECALC2 program, which reads files produced by the microprobe and assigns analyses to the relevant recalculation

TABLE 1.   Mineral-specific programs and their functions

| Mineral | Formula | Estimation of $Fe^{3+}$ | Stoichiometry check | Calculation of end-members | Reference | Normalization based on: |
|---|---|---|---|---|---|---|
| Amphibole | — | X | X | — | Spear and Kimball (1984) | 8 normalizations (see reference) |
| Spinel | $R2R3_2O_4$ | X | X | X | Finger (1972) | $\Sigma R2 = 1; \Sigma R3 = 2$ |
| Pyroxene | $M2M1T_2O_6$ | X | X | X | Papike et al. (1974) | $\Sigma M2 = 1; \Sigma M1 = 1; \Sigma T = 2$ |
| Garnet | $X_3Y_2Z_3O_{12}$ | X | X | X | — | $\Sigma R2 = Al6 + Cr + Ti + Zr + Fe^{3+}$ $+ V = 2$ |
| Feldspar | — | — | X | X | — | — |
| Olivine | — | — | X | X | — | — |
| Ilmenite | $R2R3O_3$ | X | X | X | — | $\Sigma R3 = Ti + Zr + Al + Cr + Fe^{3+}$ $+ V + Nb + Ta = 1$ |
| Carbonate | — | — | X | — | — | wt% oxide → wt% carbonate |
| Epidote | — | X | X | — | — | Total Fe = $Fe_2O_3$ |
| Chloritoid | $R2R3Al_3Si_2O_{12}$ | X | X | — | — | $\Sigma R3 = (Al-3) + Ti + Fe^{3+} + Cr = 1$ |
| Pumpellyite | $Ca_8R2_2R3_{10}Si_{12}O_{49}$ | X | X | — | — | $\Sigma R3 = Ti + Al + Cr + Fe^{3+} = 10$ |
| Sapphirine | $R2_4R3_8Si_2O_{20}$ | X | X | — | Higgins et al. (1979) | $Fe^{3+} = Al4 - (Al6 + Cr)$ |
| Mica | — | — | X | — | — | 11 O atoms, 7 cations, and 6 cations |
| Sulfide | — | — | X | — | — | — |

295

```
                                      FORMAT
A10                         [MINERAL TYPE]
1X, I5,26A1,11A1,F5.1 [#EL; SAMPLE; DESC;#OX]
1X,2A1,A2,F8.4,F7.2 (EL,;CATIONS;OXIDES]

OLIVINE
            12,OLIVINE             ,CORE ,        4.0
Si,    .9970      39.87
Ti,    .0010        .03
Al,    .0000        .00
Cr,    .0000        .00
Fe2,   .2920      13.97
Ni,    .0000        .00
Mn,    .0050        .22
Mg,   1.6920      45.38
Ca,    .0070        .25
Na,    .0000        .00
K,     .0000        .00
Cl,    .0000        .00
RECAMP
            12,KAERSUTITE          ,CORE ,       23.0
Si,   6.0180      39.89
Ti,    .6017       5.30
Al,   2.4131      13.57
Cr,    .0000        .00
Fe2,  1.6633      13.18
Ni,    .0000        .00
Mn,    .0000        .00
Mg,   2.3462      10.43
Ca,   1.5605       9.65
Na,    .8257       2.82
K,     .3162       1.64
Cl,    .0000        .00
PYROX
            12,DEL CPX             ,CORE ,        6.0
Si,   1.8952      51.34
Ti,    .0104        .38
Al,    .2209       5.08
Cr,    .0218        .75
Fe2,   .1126       3.65
Ni,    .0000        .00
Mn     .0000        .00
Mg,    .8540      15.52
Ca,    .8303      21.00
Na,    .0523        .73
K,     .0000        .00
Cl,    .0000        .00
FELDSPAR
            12, PLAGIOCLASE        ,CORE ,        8.0
Si,   2.3804      51.91
Ti,    .0000        .00
Al,   1.6059      29.71
Cr,    .0000        .00
Fe2,   .0101        .26
Ni,    .0000        .00
Mn,    .0000        .00
Mg,    .0000        .00
Ca     .6570      13.37
Na,    .3147       3.54
K,     .0121        .21
Cl,    .0000        .00
```

Fig. 1. Format and example of .EDS file from the microprobe which can be read by RECALC2.

program; (2) 14 mineral-specific recalculation programs (see Table 1); and (3) the ASSIGNPI program, which rearranges the input oxides into the correct order for each recalculation program.

**Input**

RECALC2 is menu driven. The user may choose to process .EDS files from the microprobe or use any of the mineral-specific programs entering data from the keyboard as prompted. The programs are specific to microprobe data, i.e., mineral formulae are recalculated on an anhydrous basis. The input analysis number, number of elements analyzed for each sample, sample name, sample description, and number of O atoms for cation normalization are printed on the screen as they are read, to ensure that all data are entered correctly. Each analysis is then sent to the appropriate program for recalculation. The format of the .EDS file is shown in Figure 1. Microprobe programs need to be modified to produce an .EDS file with this format before RECALC2 can be executed.

A summary of the mineral-specific recalculation programs and their functions is presented in Table 1. For minerals not covered by a specific recalculation program, the wt% oxides and cations/specified number of O atoms are calculated and listed, but no assessment of analysis quality is made.

**Output**

Three output files are produced by the RECALC package.

1. A USER. file. This file gives the full output, listing input and recalculated oxides and cations, site occupancies, ratios, and end-members. This output allows assessment of analysis quality, and can be sent to the line printer, e.g., Figure 2.

2. A USER.MAC file. This file lists information for the recalculated analyses and consists of a headerline followed by analysis data. The headerline contains the fields: sample, description, mineral type, number of O atoms, oxides analyzed, oxide total, recalculated $Fe_2O_3$, FeO and Total, cations for the recalculated analyses, cation total, Mg number, and end-members and ratios as appropriate. The format of the file is tab-delimited, text-only ASCII format, with one analysis per row after the headerline. If a mixture of minerals is analyzed, and different element lists are used, a new headerline is entered for each element list, followed by data relevant to that list. This file can be sorted (see below) and transposed to produce tables of analyses for publication.

3. A USER.RAW file. This file has a similar tab-delimited format to the USER.MAC file, and consists of a headerline with fields for sample name, description, mineral type, number of O atoms, wt% original oxides, and oxide total, followed by analytical data with one analysis per row. This file can be used as input to other programs if, for example, different cation normalizations are required.

**DATA MANIPULATION**

If only one mineral species has been analyzed, the USER.MAC and USER.RAW files can be read straight into spreadsheet packages. If more than one mineral type has been analyzed, it is useful to pass the data through a sorting program before reading into a spreadsheet. A Macintosh application, EMConvert, is available for sorting the data and producing a Mac-usable file, and a similar program could be written for IBM compatible systems. Obtaining a usable Macintosh file from the PC requires two steps: the first involves transferring the file from an IBM-PC 5.25-in. disk to a Mac 3.5-in. disk. To do this, an Apple PC 5.25-in. external Drive and Mac SE-Bus Drive Card need to be installed in a Macintosh SE. The file exchanges are then performed using Apple File Exchange which is standard system software. The second step requires writing the data in a form readable by standard Macintosh applications, i.e., tab-delimited text-only files. The EMConvert application:

1. Removes unwanted characters, e.g., linefeeds.

2. Allows sorting of the data according to sample name or mineral type.

3. Reads the data to identify all different fields in the head-

Date: 03-26-1989  E.M. CENTRE, UWA: Pyroxene recalculation program (JRM)

Sample: DEL CPX: Description: CORE

Cycles:    1 Flags: 1. Delta:0.00000 Residual: -.00273 - .00273

| | SiO2 | TiO2 | Al2O3 | Cr2O3 | Fe2O3 | FeO | MnO | MgO | CaO | Na2O | | Total |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 51.34 | .38 | 5.08 | 0.75 | 0.00 | 3.65 | 0.00 | 15.52 | 21.00 | 0.73 | | 98.45 |
| | 51.34 | .38 | 5.08 | 0.75 | 0.00 | 3.65 | 0.00 | 15.52 | 21.00 | 0.73 | | 98.45 |
| | 1.895 | 0.011 | 0.221 | 0.022 | 0.000 | 0.113 | 0.000 | 0.854 | 0.831 | 0.052 | | 3.999 |
| | 1.895 | 0.011 | 0.221 | 0.022 | 0.000 | 0.113 | 0.000 | 0.854 | 0.831 | 0.052 | | 3.999 |

| Si | 1.895 | Al6 | 0.117 | XOct | 0.116 | Quad | 85.10 | Wo | 46.22 | Ti | 6.30 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Al4 | 0.105 | Fe2 | 0.113 | Ca | 0.831 | Othr | 14.90 | En | 47.51 | NaM2 | 31.22 |
| Tet | 2.000 | Fe3 | 0.000 | Na | 0.052 | Sum | 100.00 | Fs | 6.27 | Al | 62.47 |
| | | Mg | 0.854 | M2 | 0.999 | XFe2 | 0.12 | Sum | 100.00 | Ssum | 100.00 |
| | | Mn | 0.000 | | | | | | | | |
| | | Ti | 0.011 | | | | | | | | |
| | | Cr | 0.022 | | | | | | | | |
| | | Oct | 1.116 | | | | | | | | |

SUMMARY

| | | | | |
|---|---|---|---|---|
| 1. | Tetrahedral Site (=2+-0.02) | Yes | Quad | 85.10 |
| 2. | Octahedral Cations (>.98) | Yes | Wo | 46.22 |
| 3. | XOct+Ca (<=1.01) | Yes | En | 47.51 |
| 4. | M2 Site (=1+-0.02) | Yes | Fs | 6.27 |
| 5. | Residual (<0.01) | Yes | CAALCATS | 14.90 |
| | Analysis Accepted | | Fe203 | 0.00 |
| | | | Mg/Mg+Fe2 | 88.34 |

Date: 03-26-1989    E.M. CENTRE, UWA:  Feldspar recalculation program (JRM)

Sample:PLAGIOCLASE      :      Description: CORE

| Oxides | | Cations/8 oxygens | | End-members | |
|---|---|---|---|---|---|
| SiO2 | 51.91 | Si | 2.380 | Ca/Ca+Na+K | 0.67 |
| TiO2 | 0.00 | Ti | 0.0000 | Na/Ca+Na+K | 0.32 |
| Al2O3 | 29.71 | Al | 1.606 | K/Ca+Na+K | 0.01 |
| Cr2O3 | 0.00 | Cr | 0.000 | Anorthite | 66.09 |
| Fe2O3 | 0.00 | Fe3+ | 0.000 | Albite | 31.67 |
| FeO | 0.26 | Fe2+ | 0.010 | Orthoclase | 1.24 |
| MnO | 0.00 | Mn | 0.000 | Ca/site | 0.66 |
| MgO | 0.00 | Mg | 0.000 | Na/X-site | 0.32 |
| CaO | 13.37 | Ca | 0.657 | K/X-site | 0.01 |
| Na2O | 3.54 | Na | 0.315 | | |
| K2O | 0.21 | K | 0.012 | | |
| Total | 99.00 | Total | 4.980 | | |

DATE: 03-26-1989  E.M. CENTRE UWA:     Olivine recalculation program (JRM)

Sample:         OLIVINE     Description:    CORE

| Oxides | | Cations/4 oxygens | | End-members | |
|---|---|---|---|---|---|
| SiO2 | 39.87 | Si | 1.000 | Mg/Mg+Fe | 0.85 |
| TiO2 | 0.03 | Ti | 0.001 | Fe/Mg+Fe | 0.15 |
| Al2O3 | 0.00 | Al | 0.000 | Mg/R2+ | 0.85 |
| Cr2O3 | 0.00 | Cr | 0.000 | Fe/R2+ | 0.15 |
| Fe2O3 | 0.00 | Fe3+ | 0.000 | Mn/R2+ | 0.00 |
| FeO | 13.97 | Fe2+ | 0.293 | Forsterite | 85.07 |
| MnO | 0.22 | Mn | 0.005 | Fayalite | 14.70 |
| MgO | 45.38 | Mg | 1.696 | Tephroite | 0.23 |
| CaO | 0.25 | Ca | 0.007 | | |
| Na2O | 0.00 | Na | 0.000 | | |
| K2O | 0.00 | K | 0.000 | | |
| NiO | 0.00 | Ni | 0.000 | | |
| CoO | 0.00 | Co | 0.000 | | |
| Total | 99.72 | Total | 3.000 | | |

Date: 03-26-1989         E.M. CENTRE, UWA: Amphibole recalculation program (JRM)

SAMPLE:KAERSUTITE:                        Description: CORE

Lower bound = All Fe2+       Upper Bound =       Sum Fm=13

| Weight %oxide | | | All Fe2+ | Avg Fe3+ | Sum FM =13 |
|---|---|---|---|---|---|
| SiO2 | 39.89 | Si | 6.019 | 6.009 | 5.999 |
| Al2O3 | 13.57 | Aliv | 1.981 | 1.991 | 2.001 |
| TiO2 | 5.30 | AlTot | 2.414 | 2.410 | 2.406 |
| MgO | 10.43 | Alvi | 0.433 | 0.419 | 0.405 |
| FeO | 13.18 | Ti | 0.601 | 0.600 | 0.599 |
| MnO | 0.00 | Fe3+ | 0.000 | 0.075 | 0.150 |
| CaO | 9.65 | Mg | 2.345 | 2.342 | 2.338 |
| Na2O | 2.82 | Fe2+ | 1.663 | 1.585 | 1.508 |
| K2O | 1.64 | Mn | 0.000 | 0.000 | 0.000 |
| | | SumFM | 13.042 | 13.021 | 13.000 |
| Total | 96.48 | Ca | 1.560 | 1.558 | 1.555 |
| | | NaM4 | 0.397 | 0.421 | 0.445 |
| | | NaTot | 0.825 | 0.824 | 0.822 |
| | | Na-A | 0.428 | 0.402 | 0.377 |
| | | K | 0.316 | 0.315 | 0.315 |
| | | Sum-A | 0.743 | 0.718 | 0.692 |
| | | FeO* | 13.180 | 12.564 | 11.989 |
| | | Fe2O3* | 0.000 | 0.661 | 1.323 |
| | | Total* | 96.480 | 96.525 | 96.613 |
| | | Fe3/(Fe3+Fe2)= | 0.000 | 0.045 | 0.090 |
| | | Fe2/(Fe2+Mg) = | 0.415 | 0.404 | 0.392 |

Fig. 2.   Example of full output of data from Figure 1 allowing assessment of analysis quality.

| Sample Description | OLIVINE CORE | KAERSUTITE CORE | DEL CPX CORE | PLAGIOCLASE CORE |
|---|---|---|---|---|
| Mineral | OL | AM | PX | FP |
| Ox. no | 4 | 23 | 6 | 8 |
| SiO2 | 39.87 | 39.89 | 51.34 | 51.91 |
| TiO2 | 0.03 | 5.30 | 0.38 | 0.00 |
| Al2O3 | 0.00 | 13.57 | 5.08 | 29.71 |
| Cr2O3 | 0.00 | . | 0.75 | 0.00 |
| Fe2O3 | 0.00 | 0.00 | 0.00 | 0.00 |
| FeO | 13.97 | 13.18 | 3.65 | 0.26 |
| MnO | 0.22 | 0.00 | 0.00 | 0.00 |
| MgO | 45.38 | 10.43 | 15.52 | 0.00 |
| CaO | 0.25 | 9.65 | 21.00 | 13.37 |
| Na2O | 0.00 | 2.82 | 0.73 | 3.54 |
| K2O | 0.00 | 1.64 | . | 0.21 |
| CoO | 0.00 | . | . | . |
| NiO | 0.00 | . | . | . |
| Oxide total | 99.72 | 96.48 | 98.45 | 99.00 |
| Fe2O3* | . | 0.66 | 0.00 | . |
| FeO* | . | 12.56 | 3.65 | . |
| Total* | . | 96.52 | 98.45 | . |
| Si | 1.000 | 6.009 | 1.895 | 2.380 |
| Ti | 0.001 | 0.600 | 0.011 | 0.000 |
| Al | 0.000 | 2.410 | 0.221 | 1.606 |
| Cr | 0.000 | . | 0.022 | 0.000 |
| Fe3+ | 0.000 | 0.075 | 0.000 | 0.000 |
| Fe2+ | 0.293 | 1.585 | 0.113 | 0.010 |
| Mn | 0.005 | 0.000 | 0.000 | 0.000 |
| Mg | 1.696 | 2.342 | 0.854 | 0.000 |
| Ca | 0.007 | 1.558 | 0.831 | 0.657 |
| Na | 0.000 | 0.824 | 0.052 | 0.315 |
| K | 0.000 | 0.315 | . | 0.012 |
| Co | 0.000 | . | . | . |
| Ni | 0.000 | . | . | . |
| Cation total | 3.000 | 15.718 | 3.999 | 4.980 |
| Mg No | 85.27 | 59.63 | 88.34 | . |
| Forsterite | 85.07 | . | . | . |
| Fayalite | 14.70 | . | . | . |
| Tephroite | 0.23 | . | . | . |
| Other | . | . | 14.90 | . |
| Quad | . | . | 85.10 | . |
| Wollastonite | . | . | 46.22 | . |
| Enstatite | . | . | 47.51 | . |
| Ferrosilite | . | . | 6.27 | . |
| Anorthite | . | . | . | 66.8 |
| Albite | . | . | . | 32.0 |
| Orthoclase | . | . | . | 1.2 |

Fig. 3.   Example of data from Figure 1 after processing through RECALC2 and EMConvert.

mineral, description, mineral type, number of O atoms, $SiO_2$, $TiO_2$, $Al_2O_3$, $Cr_2O_3$, $Fe_2O_3$, FeO, MnO, MgO, CaO, $Na_2O$, $K_2O$, then other oxides and halogens in order of increasing atomic number, oxide total, calculated $Fe_2O_3^*$, FeO*, Total*, cations in the same order as the oxides, cation total, Mg number, then end-members and ratios as encountered. If the data are all sulfides or metals, i.e., number of O atoms is 0, then the weight percent elements are sorted in order of increasing atomic number, followed by atomic percent elements in the same order. If both sulfides and other mineral types are present in one batch of data, the program will ask whether to sort according to the silicate or sulfide list. In general, it is not advisable to execute mixed batches through the program, as the output list becomes rather unwieldy.

5. Writes a tab-delimited, text-only output file which comprises one headerline with all identified fields, followed by the data, one analysis per line and sorted as outlined above.

The output file from EMConvert can be read or imported into popular Macintosh spreadsheet or statistic packages such as Cricketgraph, Excel, or Statview, transposed, and printed as tables (e.g., Fig. 3), or further manipulated for preparation of figures.

## AVAILABILITY

Source and executable files for the RECALC2 package are available on 5.25-in. floppy disks, and the EMConvert applica-

erlines, and merges the data into a single file, taking care of missing values, etc.

4. Sorts the fields for output. If there are no sulfide or metal analyses among the data, then the fields are sorted in the order:

tion is available on 3.5-in. floppy disks. The programs and a user manual are available on request from B. J. Griffin. A fee of US $20.00, made payable to the Electron Microscopy Centre, University of Western Australia, is required to cover disk and postage costs.

## REFERENCES CITED

Afifi, A.M., and Essene, E.J. (1988) MINFILE: A microcomputer program for storage and manipulation of chemical data on minerals. American Mineralogist, 73, 446–448.

Finger, L.W. (1972) The uncertainty in the calculated ferric iron content of a microprobe analysis. Carnegie Institution of Washington Year Book 72, 600–603.

Higgins, J.B., Ribbe, P.H., and Herd, R.K. (1979) Sapphirine I: Crystal chemical contributions. Contributions to Mineralogy and Petrology, 68, 349–356.

Papike, J.J., Cameron, K.L., and Baldwin, K. (1974) Amphiboles and pyroxenes: Characterisation of OTHER than quadrilateral components and estimates of ferric iron from microprobe data. Geological Society of America Abstracts with Programs, 6, 1053–1054.

Spear, F.S., and Kimball, K.L. (1984) RECAMP—A Fortran IV program for estimating $Fe^{3+}$ contents in amphiboles. Computers and Geosciences, 10, 317–325.