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SOFTWARE NOTICE

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

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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	$R2R3Al_5Si_2O_{12}$	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	—	—	—

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```
                                                    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.

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:

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-

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.

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