

RABBIT, AN ELECTRON MICROPROBE DATA-REDUCTION  
PROGRAM USING EMPIRICAL CORRECTIONS

by

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## ABSTRACT

RABBIT is a FORTRAN IV computer program that uses Bence-Albee empirical corrections for the reduction of electron microprobe data of silicates, oxides, sulphates, carbonates, and phosphates. RABBIT efficiently reduces large volumes of data collected on 3-11 channel microprobes.

## INTRODUCTION

RABBIT is a high volume computer program written in FORTRAN IV that is designed to reduce electron microprobe data in counts to quantitative chemical analyses in weight-percent. Refinements correct the data for instrumental drift, deadtime, and background. RABBIT uses empirical correction schemes (Bence and Albee, 1968; Albee and Ray, 1970) for matrix corrections of silicates, oxides, sulphates, carbonates, and phosphates. Data sets may contain 150 individual analyses, and any number of data sets can be processed back to back. Optional routines: 1) calculate cations/unit cell; 2) normalize any three elements in terms of their atomic proportions; and 3) print tables of analyses. RABBIT was designed to be convenient, flexible, and capable of handling large amounts of data.

## METHODS

Data Handling. A flow chart (Figure 1) will aid in the following discussions, and Table 1 defines unfamiliar terms. RABBIT can reduce data sets containing as many as 150 analyses and can reduce any number of data sets back to back. Space is allocated in RABBIT for 11 elements, but more could easily be accommodated. Up to 40 counts per unknown make up the count set for each analysis. The standard deviation of the counting statistics is computed from

$$\sigma = \left[ \sum_{i=1}^n \frac{(\bar{K} - K_i)^2}{n - 1} \right]^{1/2}$$

where  $\sigma$  = standard deviation

$\bar{K}$  = average counts of count set

$K_i$  = the value of the  $i$ th count

$n$  = number of counts in count set.

Figure 1: Flow chart for program RABBIT.

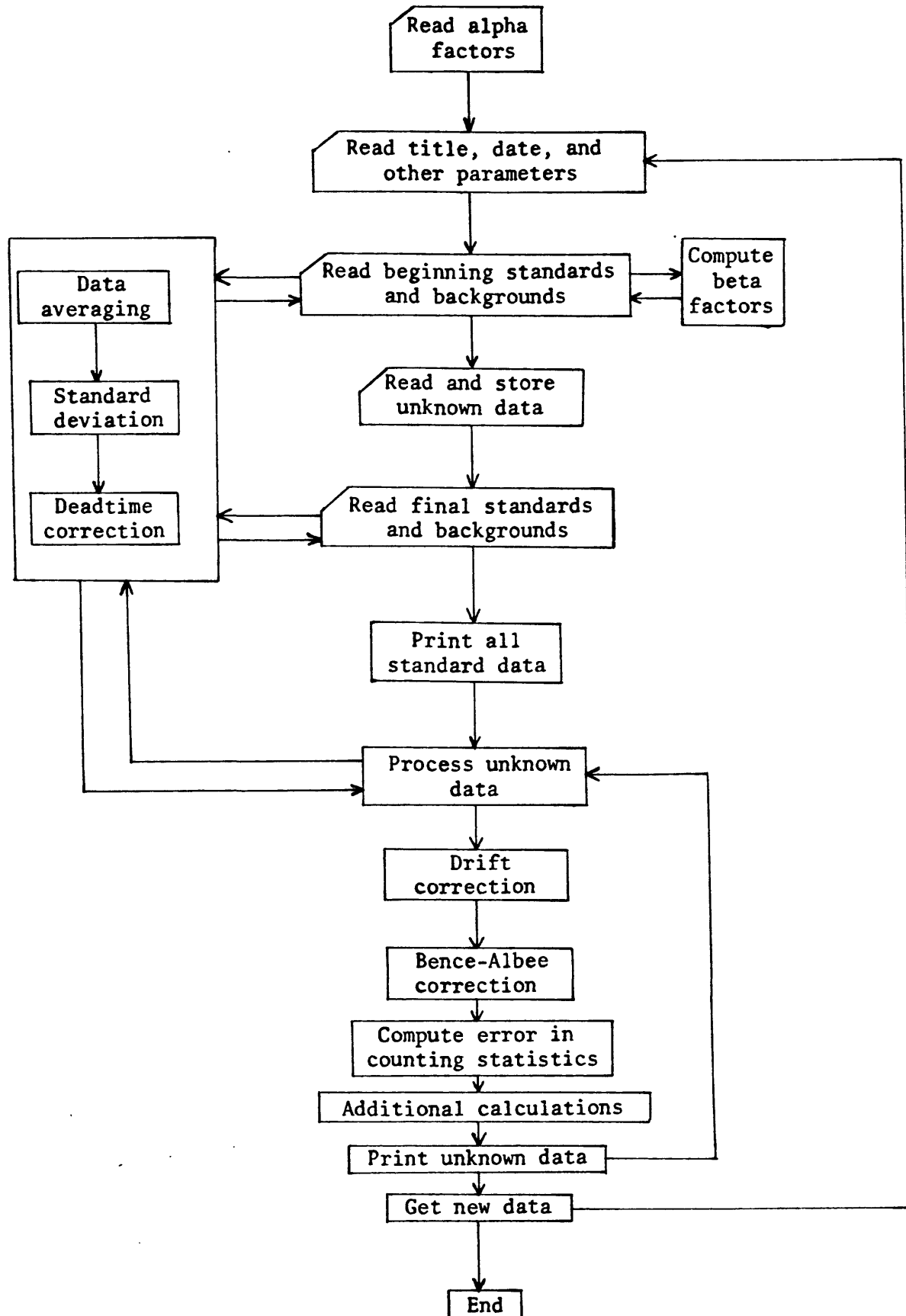


Table 1: Definition of terms

channel - the X-ray energy for each element is detected on a separate channel.

counting interval - the length of time (in sec.) that X-ray energy is counted.

counts - the energy counted during one counting interval.

count set - all the counts accumulated for each unknown; the data for one unknown makes up a count set.

data set - all the count sets accumulated for the run; the data for all the unknowns being analyzed in the run make up a data set.

run - all the data for the job; includes standard, background, and unknown data.

Deadtime. Averaged counts are next corrected for deadtime. This correction will vary from probe to probe depending on the equipment and the operating parameters in use. RABBIT is designed to function with three wavelength dispersive (WDS) channels and eight energy dispersive (EDS) channels. No deadtime correction is presently made to the three WDS channels. Counts from the EDS system are corrected for deadtime relative to the total energy stimulating the EDS detector, as measured on a ninth EDS channel. The routine that follows is adapted from Beaman and others (1972). Let

$$X_1 = \frac{E}{\bar{t}} \quad (2)$$

$$X_2 = \frac{E}{\bar{t}} (\exp(-X_1 d)) \quad (3)$$

where E = average counts from EDS system

$\bar{t}$  = average counting interval in sec.

d = deadtime of detector in sec.

For ease of manipulation we have

$$X_3 = |X_2 - X_1| \quad (4)$$

$$X_4 = X_2 Z \quad (5)$$

where Z = upper limit of convergence in sec

If  $X_3 \geq X_4$ , we make  $X_1 = X_2$  and substitute this new value of  $X_1$  into Equation (3) for iteration. The routine rapidly converges until  $X_3 < X_4$ . The counts for each individual channel are then deadtime corrected by letting

$$\bar{K}_c = \bar{K} \left( \frac{E}{\bar{t} X_2} \right) \quad (6)$$

where  $\bar{K}_c$  = deadtime corrected average counts/sec.

Values of  $d$  and  $Z$  currently built into RABBIT are  $7.5 \times 10^{-5}$  sec. and  $1.0 \times 10^{-5}$  respectively when using specimen currents less than  $3.0 \times 10^{-8}$  amp., but these values should be modified for individual needs.

Standards and Backgrounds. Standard and background data are read into the program before and after the unknown data just as they are collected on the probe. Standard and background data are averaged and deadtime corrected in the same manner as unknown data but no counting statistics are computed for backgrounds. The program reads number flags from the data cards to differentiate standards from backgrounds. Backgrounds are treated as standards which contain 0% of the unknown elements, thus background data does not need any special editing. RABBIT allows a maximum of 20 standards plus backgrounds to be used per run.

Instrument Drift and Background Corrections: Instrument drift is assumed to be linear with time. Standard and background counts are drift corrected by linear equations to the time of observation of each unknown. The standard counts are background corrected by subtracting the background counts. The unknown counts are then compared to the corrected standard counts and equated to values of weight percent. These corrections are repeated for each element to produce a raw analysis.

Bence-Albee Corrections. Because of their simplicity empirical correction schemes are used for interelement matrix effects which reduce programing costs and computer time. RABBIT incorporates the measured alpha-factors of Bence and Albee (1968) and uses the computer generated alpha-factors of Albee and Ray (1970) where measured values are not available (Table 2). The alpha-factors for 36 elements are read into the program as data and stored as a 36 x 36 matrix. The alpha factors listed in Appendix II are for probes with

a take-off angle of 52.5° and operating voltages of 15 KV. Alpha factors for other take-off angles and operating voltages may be obtained from Albee and Ray (1970). and Amlı and Griffin (1975).

Beta-factors are computed from the standards using a computer routine adapted from Eq. (3) of Albee and Ray (1970). The program allows compensation to be made for elements present in the standard which are not to be analyzed in the run. For example, if benitoite ( $\text{BaTiSi}_3\text{O}_9$ ) is used as a titanium standard, the beta-factors from benitoite must take into account the matrix effects of barium even though barium may not be included in the analysis.

Raw analyses are corrected using a computer routing following Bence and Albee (1968, p. 402) which iterates through the calculations twice.

Error in Counting Statistics. Once corrected oxide values are computed, the overall error in counting statistics is calculated from the standard deviations of counts in both standards and unknowns using partial differential equations.

We have the basic relationship

$$U = \frac{C_u S}{C_s} \quad (7)$$

where U = Unknown weight percent

S = Standard weight percent

$C_u$  = Counts of unknown

$C_s$  = Counts of standard

Because the total uncertainty of U is a function of the standard deviations of the counts for both unknown and standard,  $W_u$  and  $W_s$  (ignoring the backgrounds), the solution for the uncertainty,  $W_T$ , is obtained with partial differential



equations (for example, Holman (1966), p. 38). We have

$$W_T^2 = \left[ \left( \frac{\delta U}{\delta C_u} W_u \right)^2 + \left( \frac{\delta U}{\delta C_s} W_s \right)^2 \right] \quad (8)$$

$$\frac{\delta U}{\delta C_u} = \frac{S}{C_s} \quad (9)$$

$$\frac{\delta U}{\delta C_s} = - \frac{C_u S}{C_s^2} \quad (10)$$

$$W_T = \left[ \left( \frac{S}{C_s} W_u \right)^2 + \left( - \frac{C_u S W_s}{C_s^2} \right)^2 \right]^{\frac{1}{2}} \quad (11)$$

The final equation is used to solve for the total standard deviation.

Additional and Optional Calculations. The atom weight-percent of the elements is determined from the oxides by letting

$$W_a = \frac{(W_o f_a)}{\left( f_a + \frac{V_a 15.9994}{2.0} \right)} \quad (12)$$

where  $W_a$  = atom weight-percent of element a

$W_o$  = oxide weight-percent of element a

$f_a$  = atomic weight of element a

$V_a$  = valence of element a

Cations/unit cell (mineral norms) are calculated for all unknowns in a given data set on the same basis. Therefore, this option is best used for

runs in which all the unknowns have the same structural formula (e.g., all pyroxenes, all feldspars, etc.). We have

$$T_{ox} = T_o - T_a \quad (13)$$

$$C = \left( \frac{W_a}{f_a} \right) \left( \frac{15.9994 N_o}{T_{ox}} \right) \quad (14)$$

where  $T_{ox}$  = total weight-percent oxygen

$T_o$  = total oxide weight-percent

$C$  = cations/unit cell

$N_o$  = number of oxygens/unit cell

RABBIT will calculate the normalized atomic proportions of any three pre-chosen elements for each analysis. This option is convenient for later construction of ternary plots and is most effective when a run consists of all feldspars or all pyroxenes, etc.

Each analysis is printed with complete information on raw counts, counting statistics, raw analysis, corrected analysis, and atomic proportions. A final option prints a table of all analyses with the calculated cations/unit cell underneath.

## DECK SET-UP

A ready-to-run deck is shown diagrammatically in Figure 2. Note that the data consists of two parts: 1) the Bence-Albee alpha factors (listed in Appendix II) and 2) the parameter cards and count data which are described in the following sections (an example is listed in the second half of Appendix II).

Figure 2: Deck set-up for program RABBIT.

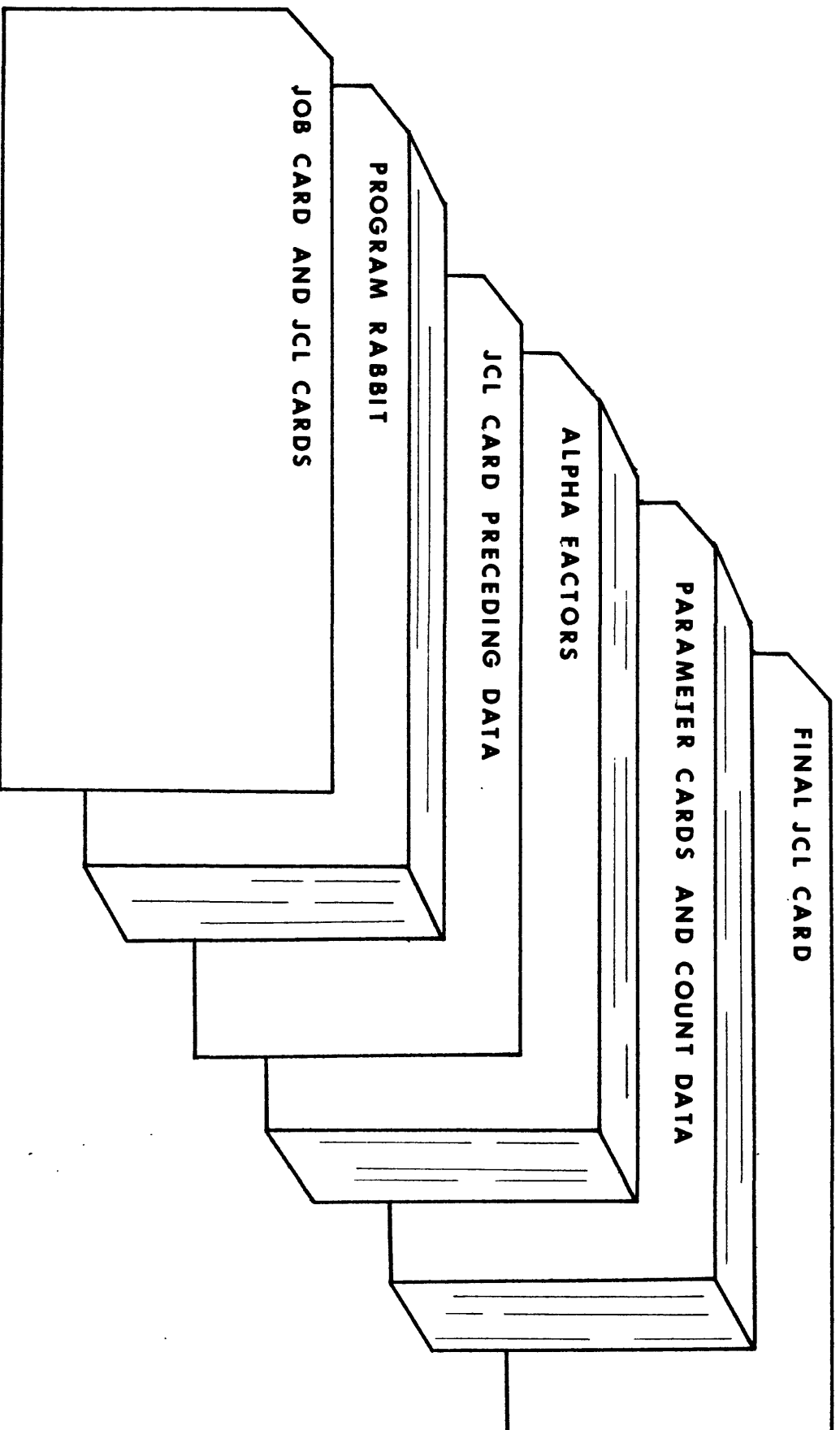


Table 2: Matrix numbers and valences of oxides and elements which can be analyzed by RABBIT (adapted from Albee and Ray, 1970).

Matrix Number	Oxide or Element	Valence	Matrix Number	Oxide or Element	Valence
1	O	2	19	CuO	2
2	CO <sub>2</sub>	2	20	ZnO	2
3	F	1	21	Rb <sub>2</sub> O	1
4	Na <sub>2</sub> O	1	22	SrO	2
5	MgO	2	23	Y <sub>2</sub> O <sub>3</sub>	3
6	Al <sub>2</sub> O <sub>3</sub>	3	24	ZrO <sub>2</sub>	4
7	SiO <sub>2</sub>	4	25	BaO	2
8	P <sub>2</sub> O <sub>5</sub>	5	26	La <sub>2</sub> O <sub>3</sub>	3
9	SO <sub>3</sub>	2	27	Ce <sub>2</sub> O <sub>3</sub>	3
10	Cl	1	28	Pr <sub>2</sub> O <sub>3</sub>	3
11	K <sub>2</sub> O	1	29	Nd <sub>2</sub> O <sub>3</sub>	3
12	CaO	2	30	Sm <sub>2</sub> O <sub>3</sub>	3
13	TiO <sub>2</sub>	4	31	Gd <sub>2</sub> O <sub>3</sub>	3
14	Cr <sub>2</sub> O <sub>3</sub>	3	32	Dy <sub>2</sub> O <sub>3</sub>	3
15	MnO	2	33	Er <sub>2</sub> O <sub>3</sub>	3
16	FeO	2	34	HfO <sub>2</sub>	4
17	CoO	2	35	ThO <sub>2</sub>	4
18	NiO	2	36	UO <sub>2</sub>	4

# PARAMETER CARD FORMATS

<u>Columns</u>	<u>Name</u>	<u>Format</u>	<u>Description</u>
<i>Card 1</i>			
1-80	LABEL	20A4	Title, any characters may be used
<i>Card 2</i>			
1-2	L	I2	Number of standards plus backgrounds, maximum = 20
3-4	M	I2	Number of elements to be analyzed, maximum = 11
5-7	N	I3	Number of unknowns to be analyzed, maximum = 150
8-11	OX	F4.1	Number of oxygens/unit cell (for example, 8.0 for feldspars); use 1.0 if option is ignored
12-13	MSTD	I2	Number of standard elements (for beta- factor calculations); maximum = 11
14-15	NORM(1)	I2	First element to be normalized for ternary plot; elements are identified by their channel number; program will accept numbers 1-11; use 0 in space 14 if option is ignored
15-17	NORM(2)	I2	Second element to be normalized for ternary plot
18-19	NORM(3)	I2	Third element to be normalized for ternary plot
20-21	ITAB	I2	Option to print analyses in tabular form; blank means <i>no</i> , 1 means <i>yes</i>
<i>Card 3</i>			
1-8	ROW(1),ATWT(1)	A2,F6.3	Element label and atomic weight for element in first channel (for example, FE55.847); an additional card must be used for elements in eleventh channel

<u>Columns</u>	<u>Name</u>	<u>Format</u>	<u>Description</u>
9-16, ..., ROW(2), ATWT(2),		A2, F6.3	Second channel - tenth channel
73-80 ... ROW(10), ATWT(10)			
<i>Card 4</i>			
1-8	ROW(11), ATWT(11)	A2, F6.3	Eleventh channel; remove this card if 10 or less elements are analyzed
<i>Card 5</i>			
1-2	MFLAG(1)	I2	Bence-Albee matrix number (from Table 1); numbers must be in same order as data are taken from microprobe. There must be as many matrix numbers as standard elements (item 5, card 2)
3-4, ...,	MFLAG(2), ...,	I2	Second matrix number - eleventh matrix number
21-22	MFLAG(11)		
<i>Card 6</i>			
1-2	VAL(1)	I2	Valences (from Table 1); must be in same order as data are taken from microprobe
3-4, ...,	VAL(2), ...,	I2	Second valence - eleventh valence
21-22	VAL(11)		
<i>Card 7</i>			
1-16	OXID2(1), OXID1(1)	A8, A8	Oxide and element headings to be used for table (for example; FEO FE ); must be in same order as data are taken from microprobe; last pair of headings must read TOTAL TOTAL; maximum number of heading pairs = 12; remove cards 7-9 if ITAB = 0 (item 9, card 2)
17-32, ...,	OXID2(2), OXID1(2),	A8, A8	Second pair - fifth pair of headings
65-80	..., OXID2(5), OXID1(5)		

<u>Columns</u>	<u>Name</u>	<u>Format</u>	<u>Description</u>
<i>Card 8</i>			
1-16, ..., 65-80	OXID2(6),OXID1(6), ...,OXID2(10),OXID1(10)	A8,A8	Sixth pair - tenth pair of headings
<i>Card 9</i>			
1-16, 17-32	OXID2(11),OXID1(11) OXID2(12),OXID1(12)	A8,A8	Eleventh and twelfth pairs of headings

#### STANDARD CARD FORMATS

<i>Card 1</i>			
1-52	HEAD	A52	Title of standard or background; any characters may be used
53-54	M1(J,1)	I2	Flag for first channel that declares how data are to be used in calculations; 0 = channel is ignored, 1 = channel is used for background, 2 = channel used for standard
55-56, ..., 57-58	M1(J,2), ..., M1(J,11)	I2	Flags for second - eleventh channels
<i>Card 2</i>			
1-6	WT(J,1)	F6.3	Oxide weight-percent of element in first channel
7-12, ..., 61-66	WT(J,2), ..., WT(J,11)	F6.3	Second - eleventh channels



<u>Columns</u>	<u>Name</u>	<u>Format</u>	<u>Description</u>
<i>Card 3</i> (Data card; must be re-formatted for different microprobes)			
1-6	DATA(NUM,1)	I6	Count data for first channel
7-8	---	--	Blank
9-14	DATA(NUM,2)	I6	Count data for second channel
15-16	---	--	Blank
17-22	DATA(NUM,3)	I6	Count data for third channel
23-24	---	--	Blank
25-30	JTIME	I6	Counting interval (in $10^{-3}$ sec)
31-32	---	--	Blank
33-38	ITIME	I6	Total beam current energy in counts
<i>Card 4</i> (Data card; must be re-formatted for different microprobes)			
1-6	DATA(NUM,4)	I6	Count data for fourth channel
7-8,	---	--	Blank
...			
57-62	DATA(NUM,11)	I6	Count data for eleventh channel
63-64	---	--	Blank
65-70	DATA(NUM,12)	I6	Total energy in counts for energy-dispersive system (for deadtime corrections)
Cards 3 and 4 are repeated for each count;      maximum = 40 counts			
<i>Cards 5 and 6</i> Two blank cards end the count data for the first standard or background. Repeat cards 1-6 for each additional standard or background; maximum = 20			

# UNKNOWN CARD FORMATS

<u>Columns</u>	<u>Name</u>	<u>Format</u>	<u>Description</u>
<i>Card 1</i>			
1-52	NAME(J,I)	13A4	Title of unknown; any characters may be used
<i>Cards 2 and 3</i>	Data cards; same format as cards 3 and 4 in Standard Card Formats above		
<i>Cards 4 and 5</i>	Blank cards; same procedure as cards 5 and 6 in Standard Card Formats above		

## STANDARD CARD FORMATS

(End of Run)

All standards and backgrounds are arranged in the same order before and after the unknowns; card format is the same as in Standard Card Formats above; the last pair of data cards ends with 4 blank cards.

## VARIABLE DESCRIPTIONS

ALPHA(36,36)	- matrix for storage of alpha-factors (element, oxide) listed in Appendix II
ATPRO(12)	- atomic proportions of elements in an unknown
ATWT(12)	- atomic weight of elements to be analyzed
AVE(12)	- average counts for each channel
BETA(12)	- beta-factors calculated for each element in an unknown
DATA(40,12)	- counts for each channel; 40 counts per channel
DEV(150,12)	- standard deviation of unknown data for each channel; maximum = 150 unknowns; values in weight percent
DIFF(40,12)	- difference between the average counts and the individual counts; used in standard deviation calculation, maximum = 40
DV(12)	- total standard deviation for each element used in Error in Counting Statistics routine
ENERGY	- total counts stimulating EDS system; used for deadtime correction
FLAG	- counter used to limit the number of iterations through Bence-Albee correction routine
HEAD(13)	- heading for standard and background identification; field is 13(A4) or 52 characters wide
IFLAG	- holds information in intermediate storage for calculation in Bence-Albee routine
INORM	- holds information in intermediate storage for calculation in ternary ratio routine
ITAB	- option variable to print data in tabular form
ITIME	- counting interval in $1 \times 10^{-3}$
JFLAG	- holds information in intermediate storage for calculation in Bence-Albee routine
JTIME	- absolute time in $1 \times 10^{-3}$ sec for use in drift correction
KK	- counter to control entry into various routines
KR(12)	- final Bence-Albee corrected weight percent for each element
KX	- counter to control the total number of unknowns printed in final output table
LABEL	- title of job being run
L	- number of standards plus backgrounds
L1	- counter used to calculate standard data at beginning and end of run; L1 = 1 at beginning; L1 = L + 1 at end

M	- number of elements (channels) to be analyzed
MF	- counter used to print final output table
MFLAG(12)	- Bence-Albee matrix number (from Table 1)
MG	- counter used to print final output table
MSTD	- number of standard elements; used for beta-factor calculation
MZ	- number of elements plus one; $MZ = M + 1$
M1(20,12)	- flags that control whether data will be used as standard, background, or ignored; standard = 2, background = 1, ignored = 0
M2	- counter to control entry into routine that calculates unknown data
N	- number of unknowns to be analyzed
NAME(150,13)	- title of unknown data; maximum = 150; field width = 13(A4)
NORM(3)	- three cations to be normalized for ternary plot (in mol-percent)
NUM	- counter whose maximum value equals the number of counts per unknown analysis
OX	- number of oxygens per unit cell
OXID1(12)	- oxide labels used in final output table
OXID2(12)	- element labels used in final output table
R	- counts in energy dispersive system during one counting interval; used for deadtime correction
ROW(12)	- element headings for each channel; used to label output
S	- average counting interval in $1 \times 10^{-3}$ sec
SBETA(12)	- standard beta factors for each element
SDEV(20,12)	- standard deviation of standard data for each element (channel); values in weight percent
SLOPE(12)	- slope determined by linear equation which measures change of standard value from beginning to end of run; used for drift correction; calculated for each element (channel)
STD(20,12)	- standard value in counts for each element
STIME(20)	- absolute time when standard data was read from microprobe
SUM(12)	- standard deviation of count data
T	- average absolute time when data was read from microprobe
TAB1(150,12)	- element values in weight percent to be printed in final output table
TAB2(150,12)	- element values in cations per unit cell to be printed in final output table

THOLD	- average absolute time of first data read from microprobe; used for drift correction
TIME(150)	- average absolute time of all unknown data
TNORM	- total of three cations in mol-percent for use in calculation of ternary plots
TOT	- total atom weight percent
TOTKR	- total oxide weight percent
TOTOX	- total oxygen in weight percent for an unknown
TOTWT	- total oxide weight percent for standards and backgrounds
T1	- counter to control THOLD
UNKWN(150,12)	- average unknown count data for each element; maximum = 150 unknowns
UKWT(13)	- average unknown data in weight percent for each element; Bence-Albee corrected
VAL(12)	- valences of elements for each channel
WT(20,12)	- oxide weight percent of each element for every standard and background
X1,...,X4	- used for calculating deadtime correction
XR(12)	- first Bence-Albee corrected values in weight percent for each element of an unknown; stored for final Bence-Albee correction on last iteration

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## APPENDIX I: PROGRAM LISTING



```

297 FORMAT (1H *32HSTANDARD COUNTS AND COMPOSITIONS*//)
      T1=0
      L1=1
      M2=0
      KK=-1
10   DO 5 J=L1,L
      C
      C   READ STANDARDS AND BACKGROUNDS
      C
      6   READ 6*HEAD*(M1(J,1),I=1,MSTD)
      C   FORMAT (13A4,12I2)
      301  READ 301*(WT(J,1),I=1,MSTD)
      C   FORMAT (12F6,3)
      C
      C   COMPUTE STANDARD BETA FACTORS
      C
      419  IF (KK) 419,104,104
      DO 422 I=1,MSTD
      IF (M1(J,I)-1) 422,422,423
      423  JFLAG = MFLAG(I)
      SBETA(I) = 0.0
      TOTWT = 0.0
      DO 424 K=1,MSTD
      IFLAG = MFLAG(K)
      SBETA(I) = WT(J,K) * ALPHA(JFLAG,IFLAG) + SBETA(I)
      TOTWT = TOTWT + WT(J,K)
      424  CONTINUE
      422  SBETA(I) = SBETA(I)/TOTWT
      C   CONTINUE
      C
      C   AVERAGING SECTION
      C
      104  DO 105 I=1,12
      AVE(I)=0.0
      SUM(I)=0.0
      105  CONTINUE
      ENERGY=0
      S=0
      T=0
      NUM=0
      109  NUM=NUM+1
      READ 110*(DATA(NUM,I),I=1,3),JTIME,ITIME
      110  FORMAT (16,4(2X,16))
      READ 111*(DATA(NUM,I),I=4,11),R
      111  FORMAT (16,8(2X,16))
      113  IF (DATA(NUM,1)) 500,112,113
      DO 114 I=1,12
      AVE(I)=AVE(I)+DATA(NUM,I)
      114  CONTINUE
      S=S+ITIME
      ENERGY=ENERGY+R
      T=T+JTIME
      GO TO 109
      112  NUM=NUM+1
      DO 115 I=1,12
      AVE(I)=AVE(I)/NUM
      115  CONTINUE
      T=T/NUM
      ENERGY=ENERGY/NUM
      S=(S/NUM)*0.001
      C

```

```

C      COMPUTE STANDARD DEVIATION OF COUNTS
C
62      IF (NUM-1) 63,63,62
        DO 69 K=1,NUM
        DO 68 I=1,M
          DIFF(NUM,I)=(AVE(I)-DATA(NUM,I))*(AVE(I)-DATA(NUM,I))
          SUM(I)=SUM(I)+DIFF(NUM,I)
68      CONTINUE
69      CONTINUE
        DO 67 I=1,M
          SUM(I)=SQRT(SUM(I)/(NUM-1))
67      CONTINUE
        GO TO 61
63      DO 66 I=1,M
          SUM(I)=0.0
66      CONTINUE
61      IF (T1) 38,38,39
38      THOLD=T
39      T1=T1+.1
C
C      APPLY DEADTIME CORRECTION TO ENERGY DISPENSIVE SYSTEM
C
        DO 160 I=1,M
          IF (I-3) 160,160,161
161      X1=ENERGY/S
165      X2=(ENERGY/S)*EXP(-X1*7.5E-05)
          X3=ABS(X2-X1)
          X4=X2+.1E-05
          IF (X3-X4) 162,163,163
163      X1=X2
          GO TO 165
162      AVE(I)=AVE(I)+((ENERGY/S)/X2)
160      CONTINUE
          IF (KK) 20,20,21
C
C      PRINT STANDARD INFORMATION
C
20      DO 32 I=1,M
          IF (M(J,I)) 30,30,31
31      STD(J,I)=AVE(I)
          SDEV(J,I)=(SUM(I)*WT(J,I))/STD(J,I)
          GO TO 32
30      STD(J,I)=0.0
          SDEV(J,I)=0.0
32      CONTINUE
          STIME(J)=T-THOLD
          IF (KK) 46,47,47
46      PRINT 45
45      FORMAT (1H0,5X,SHSTART)
          GO TO 48
47      PRINT 49
49      FORMAT (1H0,5X,BHFINISH)
48      PRINT 25,HEAD,STIME(J)
25      FORMAT (1H0,/,5X,13A4,5HTIME=,F9.3,/)
          PRINT 220,(ROW(I),I=1,MSTO)
220      FORMAT (1H,17X,12(A4,6X))
          PRINT 28,(STD(J,I),I=1,M)
28      FORMAT (1H0,11HAVE COUNTS=,12(F10.3))
          PRINT 26,(WT(J,I),I=1,MSTO)
          FORMAT (1H,11HWT PERCENT=,12(F10.3))
26      PRINT 65,(SDEV(J,I),I=1,M)

```

```

65 FORMAT (1H,11H STD DEV=.12(F10.3))
5 CONTINUE
C
C READ IN UNKNOWN DATA
C
KK=1
IF (M2) 36,36,37
36 DO 42 J=1,N
READ 40,(NAME(J,I),I=1,13)
40 FORMAT (13A4)
GO TO 104
21 DO 41 I=1,M
UNKNOWN(J,I)=AVE(I)
DEV(J,I)=SUM(I)
41 CONTINUE
TIME (J)=T-THOLD
42 CONTINUE
KK=0
M2=1
L1=L+1
L=2*L
GO TO 10
37 L=L/2
PRINT 8
8 FORMAT (1H,21HSTANDARD BETA FACTORS,/)
PRINT 4,(SBETA(I),I=1,MSTD)
4 FORMAT (1H0,11H BETA FACT=.12(F10.3),////)
C
C CALCULATE DRIFT IN STDs BY LINEAR EQUATIONS
C
DO 215 J=1,L
DO 216 I=1,M
IF (STD(J,I)) 217,217,218
218 SLOPE(J,I)=(STD(J,L,I)-STD(J,I))/(STIME(J,L)-STIME(J))
GO TO 216
217 SLOPE(J,I)=0.0
216 CONTINUE
215 CONTINUE
C
C INTERPOLATE BETWEEN STD AND BKGD VALUE. . . CALCULATE RAW COMPOSITIONS
C
PRINT 257
257 FORMAT (1H0,31HUNKNOWN COUNTS AND COMPOSITIONS,/)
DO 280 K=1,N
DO 265 I=1,M
M2=1
DO 266 J=1,L
IF (SLOPE(J,I)) 267,266,267
267 COUNT(N2)=SLOPE(J,I)*TIME(K) +STD(J,I)-SLOPE(J,I)*STIME(J)
WAIT(N2)=WT(J,I)
M2=M2+1
266 CONTINUE
SLOP=(COUNT(2)-COUNT(1))/(WAIT(2)-WAIT(1))
UKWT(I)=(UNKNOWN(K,I)-COUNT(1)+SLOP*WAIT(1))/SLOP
IF (UKWT(I)) 3,265,265
3 UKWT(I)=0.0
265 CONTINUE
C
C COMPUTE BENGE-ALBEE CORRECTED COMPOSITIONS
C
TOTKR=0.0

```

```

440 DO 440 I=1,M
      KR(I)=(UKWT(I)/SHETA(I))
      XR(I)=KR(I)
      TOTKR=KR(I) + TOTKR
440 CONTINUE
444 FLAG=0.0
      DO 445 I=1,M
        BETA(I)=0.0
445 CONTINUE
      DO 441 J=1,M
        JFLAG=MFLAG(J)
      DO 442 I=1,M
        IFLAG=MFLAG(I)
      BETA(J)=KR(I)* ALPHA(JFLAG,IFLAG) + BETA(J)
442 CONTINUE
447 BETA(J)=BETA(J)/TOTKR
441 CONTINUE
      TOTKR=0.0
      DO 443 J=1,M
        KR(J)=BETA(J) * XR(J)
      TABL(K,J)=KR(J)
      TOTKR=KR(J) + TOTKR
443 CONTINUE
      TABL(K,M+1)=TOTKR
      FLAG=FLAG + 1.0
      IF (FLAG-2.0) 444,444,446

C
C PRINT ANALYSES
C
446 PRINT 268,(NAME(K,J),J=1,13),TIME(K)
268 FORMAT (1H0,/,3X,13A,2X,5TIME=,F9.3,/)
258 PRINT 258,(ROW(I),I=1,M)
      FORMAT (1H,17X,12(A,6X))
269 PRINT 269,(UNKNOWN(K,I),I=1,M)
      FORMAT (1H0,11HAVE COUNTS=,12(F10.3))
270 PRINT 270,(UKWT(I),I=1,M)
      FORMAT (1H,11H OXIDE PER=,12(F10.3))
292 PRINT 292,(BETA(I),I=1,M)
      FORMAT (1H,11H BETA FACT=,12(F10.3))
408 PRINT 408,(KR(I),I=1,M)
      FORMAT (1H,11H B-A CORR=,12(F10.3))
272 PRINT 272,TOTKR
      FORMAT (1H,11H TOT WT PER=,F10.3)

C
C COMPUTE TOTAL STD DEVIATION W/ PARTIAL DIFFERENTIALS
C
      DO 64 J=1,L
      DO 431 I=1,M
        IF (M(J,I)-1) 432,432,433
432 GO TO 431
433 DV(I)=(WT(J,I) * DEV(K,I))/STD(J,I)**2.0 + ((UNKNOWN(K,I)
      1 * WT(J,I) * SDEV(J,I))/(STD(J,I) * STD(J,I)) **2.0
      DV(I)=SORT(DV(I))
431 CONTINUE
64 CONTINUE
      PRINT 271,(' DV(I),I=1,M)
271 FORMAT (1H0,11H STD DEV=,12(F10.3))

C
C COMPUTE ATOM-WT PERCENT, ATOM PROPOR., CATIONS/UNIT CELL (OPTIONAL)
C
      TOT=0.0

```

```

DO 409 I=1,M
  UKWT(I)=KR(I)
  UKWT(I)=(UKWT(I)*ATWT(I))/(ATWT(I)+((VAL(I)*15.9994)/2.0))
  ATPRO(I)=(UKWT(I)/ATWT(I))
  TOT=TOT+UKWT(I)
409 CONTINUE
PRINT 276,(UKWT(I),I=1,M)
276 FORMAT (1H,11H AT WT PER=12(F10.3))
PRINT 277,TOT
277 FORMAT (1H,11H TOT ATOMIC PRO=12(F10.3))
PRINT 283,(ATPRO(I),I=1,M)
283 FORMAT (1H,11H ATOMIC PRO=12(F10.5))
IF (OX) 280,280,274
274 TOTOX=(TOTKR-TOT)/(15.9994*OX)
  TAB2(K,M+1)=0.0
DO 291 I=1,M
  UKWT(I)=ATPRO(I)/TOTOX
  TAB2(K+1)=UKWT(I)
  TAB2(K,M+1)=TAB2(K,M+1)+UKWT(I)
291 CONTINUE
PRINT 412,(UKWT(I),I=1,M)
412 FORMAT (1H,11H ATOMS/CELL=12(F10.5))
C
C NORMALIZE THREE ELEMENTS FOR TERNARY DIAGRAMS
C
IF (NORM(1)) 280,280,464
464 TNORM=0.0
DO 460 I=1,3
  INORM=NORM(I)
  TNORM=TNORM+UKWT(INORM)
460 CONTINUE
IF (TNORM) 280,280,465
465 DO 461 I=1,3
  INORM=NORM(I)
  UKWT(INORM)=(UKWT(INORM)*100.0)/TNORM
461 CONTINUE
PRINT 462,(ROW(I),UKWT(INORM(I)),I=1,3)
462 FORMAT (1H,52H NORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS
11,42,1H,,F5.1,6X,42,1H,,F5.1,6X,42,1H,,F5.1)
280 CONTINUE
IF (ITAR) 720,720,721
720 GO TO 501
C
C PRINT DATA IN TABULAR FORM
C
721 MG=0
MF=-11
KX=N
710 IF (KX-12) 708,708,709
708 MF=MF+12
MG=N
709 GO TO 711
MF=MF+12
MG=MG+12
711 PRINT 700
700 FORMAT (1H,12(2X,24,))
710 PRINT 718,((NAME(K,J),J=1,2),K=MF,MG)
718 FORMAT (11X,12(2X,24,))
DO 712 I=1,MZ
PRINT 713,OXID(I),(TAR(I),K=MF,MG)
713 FORMAT (1H,1X,AH,12(F10.3))

```

```

712 CONTINUE
    PRINT 714,OX
714  FORMAT (1H0,/,1X,26HCATIONS/UNIT CELL, OXYGEN=F4,1,/)
    DO 715 I=1,MZ
      PRINT 713, OXID2(I),(TAB2(K,1)*K=MF,MG)
715  CONTINUE
      IF (KX-12) 501,501,717
717    KX= KX-12
      GO TO 710
500  STOP
      END
/*
//GO.SYSIN DD *

```



## APPENDIX II: SAMPLE DATA LISTING

The following data consist of 1) alpha factors (as described in text above) and 2) microprobe data. This example is for a run of five unknown pyroxenes using three standards and one background (assembled from several compounds as noted on title-card below). The elements were compared against the standards as follows:

Ca, Mg, Si	--	Diopside CPX-1
Fe, Mn	--	Hedenbergite C-9
Al, Ti	--	Amphibole 52-4

Calculated beta factors for amphibole 52-4 included compensation for Na and K.

The elements were read off the microprobe in the order Fe, Ca, Mg, Si, Al, Mn, Ti.

1	1.000	1.150	5.730	1.670	1.290	1.170	1.080	1.060	1.030
2	1.100	1.060	1.030	1.080	1.110	1.150	1.140	1.160	1.140
3	1.190	1.190	1.410	1.340	1.280	1.240	1.460	1.420	1.420
4	1.420	1.440	1.470	1.520	1.540	1.570	1.580	1.630	1.116
1	1.750	1.000	5.190	1.510	1.180	1.090	1.030	1.020	1.000
2	1.070	1.040	1.010	1.060	1.090	1.130	1.120	1.140	1.120
3	1.170	1.180	1.340	1.270	1.230	1.190	1.420	1.390	1.390
4	1.390	1.410	1.440	1.490	1.510	1.540	1.550	1.570	1.028
1	1.050	1.430	1.000	1.890	1.400	1.230	1.110	1.070	1.020
2	1.080	1.030	1.000	1.050	1.070	1.100	1.100	1.120	1.090
3	1.140	1.150	1.410	1.330	1.270	1.230	1.390	1.360	1.360
4	1.350	1.370	1.410	1.450	1.480	1.500	1.510	1.560	1.077
1	1.400	2.840	2.290	1.000	1.850	1.510	1.310	1.210	1.130
2	1.170	1.090	1.050	1.090	1.100	1.140	1.130	1.150	1.130
3	1.180	1.180	1.600	1.510	1.420	1.360	1.420	1.600	1.400
4	1.390	1.410	1.440	1.490	1.510	1.530	1.540	1.600	1.115
1	1.670	3.930	3.120	1.180	1.000	1.563	1.320	1.270	1.180
2	1.210	1.120	1.080	1.110	1.130	1.160	1.150	1.180	1.150
3	1.200	1.210	1.690	1.590	1.480	1.420	1.470	1.440	1.430
4	1.430	1.450	1.480	1.520	1.550	1.570	1.580	1.670	1.140
1	1.820	4.930	3.660	1.250	1.023	1.000	1.346	1.290	1.190
2	1.210	1.110	1.123	1.100	1.110	1.140	1.130	1.150	1.130
3	1.180	1.180	1.740	1.630	1.510	1.440	1.420	1.400	1.390
4	1.390	1.410	1.440	1.480	1.510	1.530	1.540	1.610	1.121
1	2.010	5.750	4.110	1.350	1.102	1.036	1.000	1.340	1.220
2	1.240	1.130	1.188	1.110	1.120	1.160	1.160	1.170	1.140
3	1.190	1.270	1.300	1.240	1.560	1.490	1.460	1.430	1.420

4	1.420	1.440	1.470	1.510	1.530	1.560	1.560	1.660	1.137
1	2.240	7.490	4.510	1.390	1.110	1.050	.990	1.000	1.250
2	1.250	1.130	1.080	1.100	1.110	1.140	1.130	1.150	1.120
3	1.170	1.180	1.270	1.210	1.180	1.150	1.420	1.390	1.390
4	1.360	1.400	1.430	1.470	1.500	1.520	1.520	1.610	1.122
1	2.480	4.600	4.650	1.460	1.160	1.080	1.020	1.010	1.000
2	1.280	1.150	1.090	1.110	1.120	1.150	1.140	1.160	1.130
3	1.180	1.190	1.320	1.250	1.210	1.170	1.450	1.420	1.410
4	1.410	1.430	1.460	1.500	1.520	1.540	1.550	1.670	1.136
1	5.950	31.460	3.260	1.190	.980	.950	.910	.920	.900
2	1.000	1.260	1.160	1.130	1.100	1.120	1.100	1.110	1.080
3	1.130	1.130	1.180	1.130	1.090	1.070	1.430	1.390	1.380
4	1.360	1.370	1.400	1.420	1.440	1.460	1.460	1.770	1.119
1	7.690	3.240	4.870	1.480	1.150	1.070	1.000	.980	.950
2	1.010	1.000	1.200	1.150	1.120	1.140	1.120	1.130	1.100
3	1.140	1.140	1.260	1.200	1.160	1.120	1.460	1.410	1.400
4	1.380	1.390	1.410	1.440	1.460	1.470	1.470	1.430	1.150
1	0.140	3.100	5.750	1.650	1.260	1.172	1.029	1.030	.990
2	1.050	.990	1.000	1.170	1.140	1.160	1.140	1.150	1.120
3	1.160	1.170	1.330	1.260	1.210	1.180	1.490	1.450	1.430
4	1.420	1.430	1.450	1.480	1.490	1.510	1.510	1.500	1.171
1	9.360	3.120	7.200	1.830	1.340	1.180	1.060	1.030	.980
2	1.020	.960	.920	1.000	1.090	1.110	1.090	1.100	1.070
3	1.110	1.110	1.320	1.250	1.190	1.150	1.290	1.270	1.270
4	1.350	1.360	1.380	1.400	1.420	1.430	1.430	1.410	1.027
1	1.670	4.180	0.700	2.140	1.500	1.280	1.120	1.060	1.000
2	1.030	.960	.910	.900	1.000	1.030	1.080	1.090	1.060
3	1.090	1.090	1.380	1.300	1.230	1.180	1.210	1.230	1.230
4	1.230	1.250	1.280	1.390	1.400	1.410	1.400	1.370	0.987
1	1.860	5.250	9.740	2.390	1.630	1.370	1.170	1.090	1.000
2	1.030	.940	.900	.890	.940	1.000	.990	1.070	1.030
3	1.070	1.060	1.400	1.320	1.240	1.190	1.190	1.160	1.160
4	1.180	1.200	1.240	1.280	1.300	1.370	1.370	1.350	0.893
1	2.040	6.070	2.320	2.620	1.760	1.460	1.190	1.130	1.040
2	1.050	.960	.920	.910	.880	.980	1.000	1.020	1.040
3	1.080	1.070	1.470	1.380	1.290	1.230	1.210	1.180	1.180
4	1.170	1.180	1.250	1.380	1.320	1.340	1.380	1.380	0.914
1	2.180	6.960	2.340	2.860	1.890	1.530	1.270	1.160	1.050
2	1.050	.960	.910	.900	.870	.860	.940	1.000	.980
3	1.060	1.050	1.510	1.410	1.310	1.250	1.190	1.160	1.150
4	1.140	1.160	1.180	1.250	1.290	1.310	1.360	1.350	0.909
1	2.430	0.170	2.500	3.180	2.070	1.650	1.350	1.220	1.100
2	1.100	.990	.940	.940	.910	.900	.840	.970	1.000
3	1.040	1.080	1.600	1.490	1.380	1.310	1.230	1.200	1.190
4	1.180	1.190	1.210	1.240	1.310	1.340	1.350	1.410	0.942
1	2.600	9.500	2.510	2.980	2.180	1.720	1.380	1.230	1.090
2	1.080	.960	.910	.910	.890	.880	.830	.800	.900
3	1.000	1.000	1.620	1.500	1.390	1.310	1.180	1.150	1.140
4	1.140	1.150	1.160	1.190	1.200	1.270	1.290	1.350	0.916
1	2.860	1.110	2.620	2.450	2.360	1.830	1.330	1.280	1.120
2	1.100	.970	.920	.920	.900	.850	.830	.750	
3	.930	1.000	1.690	1.570	1.440	1.350	1.180	1.150	1.150
4	1.140	1.150	1.170	1.190	1.200	1.200	1.270	1.360	0.924
1	5.720	21.820	3.510	1.200	.930	.880	.820	1.570	1.390
2	1.250	1.030	.940	.920	.900	.910	.900	.910	.890
3	.920	.920	1.000	1.600	1.740	1.600	1.130	1.090	1.080
4	1.080	1.080	1.100	1.120	1.130	1.150	1.160	1.370	0.925
1	6.260	18.140	4.060	1.320	1.000	.940	.860	1.650	1.460
2	1.300	1.060	.970	.950	.920	.940	.920	.930	.910
3	.940	.940	1.040	1.000	.960	1.650	1.160	1.120	1.110
4	1.100	1.110	1.120	1.150	1.160	1.170	1.180	1.410	0.948

1 6.490.14.660. 4.450. 1.380. 1.050. .970. .890. .880. 1.350.  
 2 1.330. 1.080. .990. .960. .940. .960. .940. .950. .930.  
 3 .960. .970. 1.090. 1.040. 1.000. .970. 1.190. 1.150. 1.150.  
 4 1.130. 1.140. 1.160. 1.180. 1.200. 1.210. 1.220. 1.440. 0.968.  
 1 7.010.16.340. 4.960. 1.480. 1.110. 1.020. .924. .910. 1.410.  
 2 1.370. 1.110. 1.020. .980. .960. .970. .960. .970. .940.  
 3 .980. .980. 1.120. 1.070. 1.030. 1.000. 1.210. 1.180. 1.170.  
 4 1.160. 1.160. 1.180. 1.200. 1.220. 1.230. 1.240. 1.490. 0.987.  
 1 2.560. 7.380. 2.120. 1.950. 1.730. 1.610. 1.260. 1.150. .990.  
 2 .950. .840. .780. .820. .900. .930. .910. .900. .870.  
 3 .890. .890. 1.480. 1.360. 1.270. 1.180. 1.000. .980. .970.  
 4 .970. .980. 1.110. 1.130. 1.120. 1.110. 1.110. 0.638.  
 1 2.570. 7.070. 2.270. 1.960. 1.740. 1.590. 1.260. 1.140. .990.  
 2 .970. .850. .790. .800. .840. .940. .920. .920. .880.  
 3 .910. .900. 1.530. 1.400. 1.290. 1.210. 1.030. 1.000. 1.000.  
 4 .990. 1.000. 1.090. 1.130. 1.150. 1.150. 1.140. 1.140. 0.851.  
 1 2.660. 7.440. 2.320. 2.100. 1.580. 1.650. 1.300. 1.170. 1.010.  
 2 .980. .860. .800. .810. .840. .910. .910. .920. .880.  
 3 .910. .900. 1.580. 1.440. 1.330. 1.240. 1.010. 1.000. 1.000.  
 4 .990. 1.010. 1.020. 1.110. 1.140. 1.150. 1.150. 1.160. 0.851.  
 1 2.760. 7.840. 2.380. 2.190. 1.640. 1.550. 1.340. 1.200. 1.040.  
 2 1.000. .870. .810. .780. .840. .860. .890. .930. .890.  
 3 .910. .910. 1.630. 1.480. 1.360. 1.270. 1.020. .990. 1.010.  
 4 1.000. 1.010. 1.030. 1.110. 1.150. 1.160. 1.150. 1.170. 0.815.  
 1 2.830. 8.210. 2.400. 2.260. 1.520. 1.590. 1.370. 1.220. 1.040.  
 2 1.000. .870. .810. .780. .830. .850. .880. .910. .880.  
 3 .900. .900. 1.660. 1.510. 1.390. 1.280. 1.010. .980. 1.000.  
 4 .990. 1.000. 1.020. 1.040. 1.110. 1.130. 1.130. 1.170. 0.813.  
 1 2.990. 8.970. 2.460. 1.000. 1.500. 1.480. 1.430. 1.270. 1.070.  
 2 1.010. .870. .810. .780. .830. .870. .820. .870. .860.  
 3 .890. .880. 1.590. 1.570. 1.440. 1.320. .970. .950. .960.  
 4 .960. .980. 1.000. 1.020. 1.040. 1.090. 1.120. 1.170. 0.764.  
 1 3.160. .980. 2.530. 1.010. 1.690. 1.400. 1.360. 1.310. 1.090.  
 2 1.020. .870. .800. .770. .720. .770. .800. .810. .820.  
 3 .860. .860. 1.650. 1.490. 1.490. 1.360. .960. .930. .930.  
 4 .920. .950. .980. 1.000. 1.010. 1.030. 1.070. 1.160. 0.762.  
 1 3.350.10.820. 2.600. 1.030. .830. 1.470. 1.260. 1.250. 1.120.  
 2 1.040. .880. .800. .770. .730. .770. .740. .800. .780.  
 3 .840. .840. 1.540. 1.400. 1.420. 1.300. .960. .930. .920.  
 4 .900. .910. .950. .960. 1.000. 1.010. 1.050. 1.170. 0.766.  
 1 3.510.11.680. 2.680. 1.040. .840. 1.550. 1.210. 1.300. 1.160.  
 2 1.060. .880. .810. .780. .730. .720. .750. .740. .770.  
 3 .800. .820. 1.480. 1.340. 1.340. 1.350. .960. .930. .910.  
 4 .900. .900. .910. .950. .960. 1.000. 1.010. 1.180. 0.770.  
 1 4.030.14.990. 3.050. 1.140. .890. .850. 1.360. 1.210. 1.080.  
 2 1.130. .930. .840. .800. .750. .740. .710. .680. .720.  
 3 .720. .790. 1.100. 1.460. 1.350. 1.240. .970. .940. .930.  
 4 .910. .910. .920. .930. .930. .970. 1.000. 1.220. 0.790.  
 1 .570.35.330. 4.840. 1.650. 1.200. 1.120. .960. .850. .850.  
 2 .850. .800. .940. .910. .910. .880. .850. .850. .820.  
 3 .840. .840. 1.150. 1.070. 1.030. .980. 1.080. 1.050. 1.070.  
 4 1.050. 1.070. 1.050. 1.050. 1.050. 1.050. 1.040. 1.000. 0.932.  
 112.453. 3.708. 8.144. 1.960. 1.400. 1.215. 1.077. 1.028. 0.971.  
 2 1.011. 0.941. 0.894. 0.958. 0.992. 1.095. 1.069. 1.078. 1.045.  
 3 1.084. 1.083. 1.330. 1.256. 1.190. 1.147. 1.236. 1.222. 1.222.  
 4 1.219. 1.237. 1.348. 1.370. 1.382. 1.392. 1.391. 1.346. 1.000.  
 PYROXENES OF 15 DEC 751 15 KV .03 MA SECOND BATCH  
 4 7 29 6.0 9 1 2 3 1  
 F55.847CA40.08 MG24.312S128.086AL26.981MNS4.938T147.90 NA22.990K 39.102  
 1612 5 7 61513 411  
 2 2 2 4 3 2 4 1 1

FE MN	FFO MNO	CA TI	CAU T102	MG TOTAL	MGO TOTAL	SI	S102	AL	AL203
D10PSTDE CPM-1									
2.92	24.56	16.93	53.93	0.66	0.0	0.23	0.22	0.22	0 2 2 2 0 0 0
000813	011196	0007520	119230	010061	000000	000000	000000	021534	
005122	000814	000138	000339	000000	000000	000000	000000	021534	
000760	011302	007618	119243	010061	000000	000000	000000	021505	
005180	000847	000160	000313	000000	000000	000000	000000	021505	
000809	011134	007592	119258	010055	000000	000000	000000	021638	
005254	000828	000152	000310	000000	000000	000000	000000	021638	
008333	011146	007445	119271	009995	000000	000000	000000	021673	
005222	000792	000146	000311	000000	000000	000000	000000	021673	
000815	011113	007564	119287	010014	000000	000000	000000	021477	
005243	000838	000139	000295	000000	000000	000000	000000	021477	
000799	011196	007734	119299	010021	000000	000000	000000	021846	
005319	000799	000155	000304	009996	000000	000000	000000	021846	
000756	011127	007530	119314	009996	000000	000000	000000	021445	
005161	000795	000150	000354	000000	000000	000000	000000	021445	
000790	011034	007460	119329	010023	000000	000000	000000	021776	
005284	000828	000140	000320	000000	000000	000000	000000	021776	
000784	011250	007752	119342	010055	000000	000000	000000	021532	
005109	000810	000145	000312	000000	000000	000000	000000	021532	
000762	011122	007749	119358	010010	000000	000000	000000	021538	
005265	000837	000131	000310	000000	000000	000000	000000	021538	

HEDEBERGITE C-9									
24.29	21.30	1.06	48.34	0.3	3.70	0.0	0.14	0.0	2 0 0 0 2 0 0
006589	010696	000585	119418	010044	000000	000000	000000	021703	
004751	000705	000242	000322	000000	000000	000000	000000	021703	
006462	010771	000674	119432	010091	000000	000000	000000	021766	
004763	000715	000281	000337	000000	000000	000000	000000	021766	
006092	010980	000707	119444	010077	000000	000000	000000	021572	
004831	000644	000297	000334	000000	000000	000000	000000	021572	
006452	010772	000665	119456	010071	000000	000000	000000	021598	
004652	000711	000261	000323	000000	000000	000000	000000	021598	
006036	010293	000708	119469	010071	000000	000000	000000	021677	
004732	000713	000364	000335	000000	000000	000000	000000	021677	
006509	010469	000688	119485	010064	000000	000000	000000	021569	
004782	000693	000261	000321	000000	000000	000000	000000	021569	
006260	010900	000588	119498	010028	000000	000000	000000	021784	
004797	000698	000320	000340	000000	000000	000000	000000	021784	
006684	010851	000682	119511	010072	000000	000000	000000	021670	
004695	000691	000277	000335	000000	000000	000000	000000	021380	
006370	009904	000543	119528	010046	000000	000000	000000	021380	
004698	000812	000225	000328	000000	000000	000000	000000	021380	
006337	010618	000514	119543	010056	000000	000000	000000	021345	
004540	000827	000255	000336	000000	000000	000000	000000	021345	
005899	010481	000761	119557	010025	000000	000000	000000	021623	
004711	000751	000297	000343	000000	000000	000000	000000	021623	
006298	010283	000418	119570	010043	000000	000000	000000	021383	
004643	000761	000253	000383	000000	000000	000000	000000	021383	
006440	010508	000464	119582	010026	000000	000000	000000	021579	
004662	000799	000252	000352	000000	000000	000000	000000	021579	

AMPHIBULE 52-4									
26.28	10.50	4.29	39.50	10.10	0.56	3.08	2.24	1.45	0 0 0 2 0 2 2
006889	004941	001794	119609	010125	000000	000000	000000	020144	
004100	001353	000192	000485	000000	000000	000000	000000	020144	
007016	005167	001810	119621	010088	000000	000000	000000	020144	

004055	001375	000197	000429	000000	000000	000000	000000	000000	020154
006948	005010	001882	119634	010067	000000	000000	000000	000000	020199
004057	001343	000201	000449	000000	000000	000000	000000	000000	020199
006973	005097	001905	119646	010043	000000	000000	000000	000000	020129
004036	001332	000185	000464	000000	000000	000000	000000	000000	020129
006735	005137	001748	119659	010038	000000	000000	000000	000000	019863
003905	001342	000167	000502	000000	000000	000000	000000	000000	019863
006993	005193	001724	119671	009990	000000	000000	000000	000000	020066
004012	001289	000190	000463	000000	000000	000000	000000	000000	019945
007161	005217	001913	119684	010021	000000	000000	000000	000000	019945
004035	001300	000212	000419	000000	000000	000000	000000	000000	020197
006980	005024	001842	119696	010034	000000	000000	000000	000000	020197
003978	001357	000185	000464	000000	000000	000000	000000	000000	020056
007040	005020	001752	119709	010023	000000	000000	000000	000000	020056
003978	001420	000214	000456	000000	000000	000000	000000	000000	020056
006803	005142	001795	119721	010059	000000	000000	000000	000000	020053
003986	001325	000168	000492	000000	000000	000000	000000	000000	020053

BACKGROUNDS OFF AL2O3, SiO2, AND CPX-1

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.1	1.1	1.1	1.1	1.1	1.1
51	118	59	119800	10023	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
548	822	146	298											20100

CR2S1 BEGIN ANALYSES OF SECOND GROUP OF PYROXENES

003507	008773	005273	119818	010135	000000	000000	000000	000000	020645
004727	000929	000153	000398	000000	000000	000000	000000	000000	020645
003462	008858	005254	119831	010050	000000	000000	000000	000000	020741
004594	000961	000172	000405	000000	000000	000000	000000	000000	020741
003420	008734	005467	119843	010123	000000	000000	000000	000000	020506
004721	000910	000176	000354	000000	000000	000000	000000	000000	020506
003438	008650	005397	119856	010109	000000	000000	000000	000000	020945
004791	000904	000161	000419	000000	000000	000000	000000	000000	020945

66	004027	008470	005324	119875	010081	000000	000000	000000	020946
004836	000886	000164	000359	000000	000000	000000	000000	000000	020946
004235	008105	005275	119889	010088	000000	000000	000000	000000	020775
004877	000900	000179	000352	000000	000000	000000	000000	000000	020775
004113	008093	005310	119903	010098	000000	000000	000000	000000	021026
004934	000828	000172	000385	000000	000000	000000	000000	000000	021026
004277	008080	005182	119916	010091	000000	000000	000000	000000	020813
004824	000838	000160	000369	000000	000000	000000	000000	000000	020813

67	003557	008529	005655	119940	010081	000000	000000	000000	020657
004836	000905	000161	000387	000000	000000	000000	000000	000000	020657
003571	008451	005655	119955	010089	000000	000000	000000	000000	020549
004699	000873	000142	000415	000000	000000	000000	000000	000000	020549

68	003621	008704	005575	120022	010057	000000	000000	000000	020643
004797	000861	000171	000400	000000	000000	000000	000000	000000	020741
003751	008109	005692	120036	010060	000000	000000	000000	000000	020741
004809	000902	000188	000390	000000	000000	000000	000000	000000	020819
003747	008414	005612	120048	010021	000000	000000	000000	000000	020819
004771	000975	000179	000394	000000	000000	000000	000000	000000	020819



006519	010243	000471	122357	010076	000000	000000	000000	021373
004630	000851	000237	000341	000000	000000	000000	000000	021373
006434	010194	000434	122370	010065	000000	000000	000000	021677
004704	000746	000275	000345	000000	000000	000000	000000	021677
006409	010339	000492	122382	010053	000000	000000	000000	021517
004665	000838	000252	000335	000000	000000	000000	000000	021517
006429	010354	000490	122395	010049	000000	000000	000000	021489
004671	000773	000226	000337	000000	000000	000000	000000	021489

AMPHIBOLE 52-4

26.28	10.56	4.29	39.50	10.10	0.56	3.08	2.24	1.45	0	0	0	2	0	2	2
006937	005041	001724	122422	010052	000000	000000	000000	000000	019855						
003916	001392	000215	000507	000000	000000	000000	000000	000000	019855						
007118	005102	001702	122434	010045	000000	000000	000000	000000	020151						
004058	001358	000159	000463	000000	000000	000000	000000	000000	020151						
007039	005014	001770	122447	010049	000000	000000	000000	000000	020125						
004034	001358	000188	000426	000000	000000	000000	000000	000000	020125						
006992	005004	001766	122459	010073	000000	000000	000000	000000	020201						
003962	001375	000209	000424	000000	000000	000000	000000	000000	020201						
006945	005107	001807	122472	010048	000000	000000	000000	000000	020056						
003985	001391	000194	000488	000000	000000	000000	000000	000000	020056						
007038	005002	001926	122485	010026	000000	000000	000000	000000	019953						
004059	001279	000191	000457	000000	000000	000000	000000	000000	019953						
006977	004998	001720	122498	010000	000000	000000	000000	000000	019909						
003844	001297	000187	000507	000000	000000	000000	000000	000000	019909						
007170	004977	001682	122522	010030	000000	000000	000000	000000	020013						
003989	001299	000209	000491	000000	000000	000000	000000	000000	020013						
007165	004918	001893	122535	010023	000000	000000	000000	000000	019924						
003943	001342	000197	000442	000000	000000	000000	000000	000000	019924						
007013	005036	001920	122547	009997	000000	000000	000000	000000	019984						
003934	001321	000207	000452	000000	000000	000000	000000	000000	019984						
007032	005201	001911	122559	010031	000000	000000	000000	000000	019671						
003873	001361	000165	000435	000000	000000	000000	000000	000000	019671						

BACKGROUNDS OFF AL2O3, SiO2, AND CPX-1

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	1	1	1	1	1	1
50	120	60	122650	10023											
550	821	147	299												20100



### APPENDIX III: SAMPLE OUTPUT LISTING

NO. STDS= 4 NO. ELEM= 7 NO. UNKNOWN= 5 NO. STU ELEM= 9 NO. OXYGENS= 6.0

STANDARD COUNTS AND COMPOSITIONS

START

DIOPSIDE CPX-1

FE

CA

MG

SI

AL

MN

TI

NA

K

TIME= 0.0

AVE COUNTS= 0.0  
WT PERCENT= 2.920  
STD DEV= 0.0

11162.000  
24.560  
0.093

7596.398  
16.930  
0.358

6001.824  
53.930  
0.465

0.0  
0.660  
0.0

0.0  
0.0  
0.0

0.0  
0.230  
0.0

0.220

0.220

START

WEDENBERGITE C-9

FE

CA

MG

SI

AL

MN

TI

NA

K

TIME= 206.375

AVE COUNTS= 6340.613  
WT PERCENT= 24.290  
STD DEV= 0.396

0.0  
21.300  
0.0

0.0  
1.060  
0.0

0.0  
48.340  
0.0

0.0  
0.300  
0.0

317.207  
3.700  
0.289

0.0  
0.0  
0.0

0.140

0.0

START

AMPHIBOLE 52-4

FE

CA

MG

SI

AL

MN

TI

NA

K

TIME= 371.938

AVE COUNTS= 0.0  
WT PERCENT= 26.280  
STD DEV= 0.0

0.0  
10.500  
0.0

0.0  
4.290  
0.0

0.0  
39.500  
0.0

1532.412  
10.100  
0.130

0.0  
0.560  
0.0

527.226  
3.080  
0.183

2.240

1.450

START

BACKGROUNDS OFF AL2O3, SiO2, AND CPX-1

TIME= 506.938

FE

CA

MG

SI

AL

MN

TI

NA

K

AVE COUNTS= 51.000  
WT PERCENT= 0.0  
STD DEV= 0.0

118.000  
0.0  
0.0

59.000  
0.0  
0.0

625.219  
0.0  
0.0

937.829  
0.0  
0.0

166.573  
0.0  
0.0

339.991  
0.0  
0.0

0.0

0.0

FINISH

DIOPSIDE CPX-1

FE

CA

MG

SI

AL

MN

TI

NA

K

TIME= 2801.063

AVE COUNTS= 0.0  
WT PERCENT= 2.920

11161.250  
24.560

7550.414  
16.930

5992.934  
53.930

0.0  
0.660

0.0  
0.0

0.0  
0.230

0.220

0.220

STD DEV= 0.0 0.220 0.102 0.481 0.0 0.0 0.0

FINISH

MEDEBERGITE C-9

TIME= 3015.813

	FE	CA	MG	SI	AL	MN	TI	NA	K
AVE COUNTS=	6402.426	0.0	0.0	0.0	0.0	324.486	0.0		
WT PERCENT=	24.290	21.300	1.060	48.340	0.300	3.700	0.0	0.140	0.0
STD DEV=	0.105	0.0	0.0	0.0	0.0	0.665	0.0		

FINISH

AMPHIBOLE 52-4

TIME= 3196.000

	FE	CA	MG	SI	AL	MN	TI	NA	K
AVE COUNTS=	0.0	0.0	0.0	0.0	1531.033	0.0	527.721		
WT PERCENT=	26.280	10.500	4.290	39.500	10.100	0.560	3.080	2.240	1.450
STD DEV=	0.0	0.0	0.0	0.0	0.125	0.0	0.171		

FINISH

BACKGROUNDS OFF AL2O3, SiO2, AND CPX-1

TIME= 3356.938

	FE	CA	MG	SI	AL	MN	TI	NA	K
AVE COUNTS=	50.000	120.000	60.000	627.501	936.688	167.714	341.132		
WT PERCENT=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
STD DEV=	0.0	0.0	0.0	0.0	0.0	0.0	0.0		

## STANDARD BETA FACTORS

BETA FACT= 1.110 1.114 1.145 1.070 1.201 1.110 1.057 1.720 1.058  
UNKNOWN COUNTS AND COMPOSITIONS

## CR2S1 BEGIN ANALYSES OF SECOND GROUP OF PYROXENES TIME= 543.938

	FE	CA	MG	SI	AL	MN	TI
AVE COUNTS=	3456.750	8763.750	5352.750	5385.453	1059.190	189.305	450.670
OXIDE PER=	13.137	19.227	11.905	47.763	2.062	0.555	1.820
BETA FACT=	1.130	1.093	1.215	1.082	1.192	1.133	1.091
B-A CORR=	13.375	18.859	12.640	48.309	2.047	0.566	1.878
TOT WT PER=	97.674						

STD DEVI=	0.083	0.187	0.114	0.859	0.167	0.061	0.169
AT WT PER=	10.396	13.479	7.623	22.582	1.083	0.439	1.126
TOT ATOMPC=	56.727	0.33630	0.31356	0.80401	0.04015	0.00798	0.02350
ATOMIC PRO=	0.18616	0.78843	0.73511	1.88496	0.09412	0.01872	0.05510
ATOMS/CELL=	0.43643						

NORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS:FE, 22.3 CA, 40.2 MG, 37.5

## 66 TIME= 602.688

	FE	CA	MG	SI	AL	MN	TI
AVE COUNTS=	4163.000	8187.000	5272.750	5574.625	988.321	193.255	419.435
OXIDE PER=	15.858	17.944	11.726	49.663	0.858	0.650	1.306
BETA FACT=	1.127	1.091	1.230	1.081	1.200	1.129	1.085
B-A CORR=	16.101	17.579	12.597	50.186	0.857	0.661	1.341
TOT WT PER=	99.323						

STD DEVI=	0.504	0.272	0.234	0.454	0.190	0.118	0.019
AT WT PER=	12.516	12.564	7.598	23.459	0.454	0.512	0.804
TOT ATOMPC=	57.906	0.31347	0.31250	0.83525	0.01681	0.00932	0.01678
ATOMIC PRO=	0.22411	0.72657	0.72431	1.93592	0.03897	0.02161	0.03889
ATOMS/CELL=	0.51943						

NORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS:FE, 26.4 CA, 36.9 MG, 36.8

## 67 TIME= 654.438

	FE	CA	MG	SI	AL	MN	TI
AVE COUNTS=	3564.000	8490.000	5655.000	5451.141	1016.479	173.225	458.502
OXIDE PER=	13.546	18.618	12.587	48.425	1.337	0.161	1.949
BETA FACT=	1.130	1.094	1.215	1.082	1.196	1.133	1.090
B-A CORR=	13.794	18.274	13.360	48.963	1.331	0.164	2.010
TOT WT PER=	97.896						

STD DEVI=	0.038	0.121	0.001	0.870	0.149	0.157	0.116
AT WT PER=	10.722	13.060	8.058	22.887	0.705	0.127	1.205
TOT ATOMPC=	56.764	0.32586	0.33143	0.81491	0.02611	0.00231	0.02515
ATOMIC PRO=	0.19199						

ATOMS/CELL= 0.44807 0.76050 0.77349 1.90186 0.06094 0.00540 0.05870  
 NORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS:FE, 22.6 CA, 38.4 MG, 39.0

68

FE CA MG SI AL MN TI  
 TIME= 742.250

AVE COUNTS= 3706.333 8409.000 5626.332 5486.188 1044.807 205.298 451.808  
 OXIDE PER= 14.090 18.438 12.525 48.779 1.819 0.941 1.838  
 BETA FACT= 1.129 1.092 1.220 1.084 1.197 1.131 1.088  
 B-A CORR= 14.327 18.072 13.344 49.425 1.813 0.959 1.891  
 TOT WT PER= 99.832

STD DEV= 0.191 0.013 0.039 0.235 0.503 0.005 0.005  
 AT WT PER= 11.137 12.916 8.048 23.103 0.959 0.743 1.134  
 TOT ATOMP= 58.040  
 ATOMIC PRO= 0.11942 0.32226 0.33103 0.82258 0.03556 0.01352 0.02367  
 ATOMS/CELL= 0.45806 0.74025 0.76038 1.88949 0.08167 0.03105 0.05437

NORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS:FE, 23.4 CA, 37.8 MG, 38.8

69

FE CA MG SI AL MN TI  
 TIME= 812.563

AVE COUNTS= 3486.667 8750.000 5401.664 5480.316 1086.362 183.352 463.728  
 OXIDE PER= 13.240 19.196 12.022 48.722 2.526 0.405 2.034  
 BETA FACT= 1.130 1.094 1.213 1.083 1.190 1.133 1.091  
 B-A CORR= 13.483 18.843 12.743 49.305 2.502 0.414 2.099  
 TOT WT PER= 99.390

STD DEV= 0.604 0.798 0.178 0.008 0.137 0.057 0.219  
 AT WT PER= 10.481 13.467 7.685 23.047 1.324 0.320 1.258  
 TOT ATOMP= 57.584  
 ATOMIC PRO= 0.18767 0.33601 0.31611 0.82060 0.04909 0.00583 0.02626  
 ATOMS/CELL= 0.43093 0.77157 0.72586 1.88428 0.11271 0.01340 0.06031

NORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS:FE, 22.3 CA, 40.0 MG, 37.6

	CR2S1 R	66	67	68	69
FE0	13.375	16.101	13.794	14.327	13.483
CA0	14.859	17.579	18.274	18.072	18.843
MG0	12.640	12.597	13.360	13.344	12.743
SI02	48.309	50.186	48.963	49.425	49.305
AL203	2.047	0.857	1.331	1.813	2.502
MNO	0.566	0.661	0.164	0.959	0.414
TIO2	1.878	1.341	2.010	1.691	2.099
TOTAL	97.674	99.323	97.896	99.832	99.390

CATIONS/UNIT CELL: OXYGEN= 6.0

FE	0.436	0.519	0.448	0.458	0.431
CA	0.788	0.727	0.760	0.740	0.772
MG	0.735	0.724	0.773	0.760	0.726
SI	1.885	1.936	1.902	1.889	1.884
AL	0.094	0.039	0.061	0.082	0.113
MN	0.019	0.022	0.005	0.031	0.013
TI	0.055	0.039	0.059	0.054	0.060
TOTAL	4.013	4.006	4.009	4.015	3.999