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 ith count

\( n \) = number of counts in count set.
Figure 1: Flow chart for program RABBIT.

1. Read alpha factors
2. Read title, date, and other parameters
3. Read beginning standards and backgrounds
4. Read and store unknown data
5. Read final standards and backgrounds
6. Print all standard data
7. Process unknown data
8. Drift correction
9. Bence-Albee correction
10. Compute error in counting statistics
11. Additional calculations
12. Print unknown data
13. Get new data
14. End
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

\[ X_1 = \frac{E}{\bar{t}} \]  
\[ X_2 = \frac{E}{\bar{t}} \left( \exp \left( -X_1 d \right) \right) \]  

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

\[ X_3 = \left| X_2 - X_1 \right| \]  
\[ X_4 = X_2 Z \]  

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

\[ \overline{K}_c = K \left( \frac{E}{X_2} \right) \]  

where \( \overline{K}_c \) = 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 $36 \times 36$ 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 Amli 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 (BaTiSi_3O_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

\[ U = \frac{C_u S}{C_s} \]  

(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

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

(8)

\[
\frac{\partial U}{\partial C_u} = \frac{S}{C_s}
\]

(9)

\[
\frac{\partial U}{\partial C_s} = -\frac{C_u S}{C_s^2}
\]

(10)

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

(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

\[
W_a = \frac{(W_o f_a)}{\left( f_a + V_a \frac{15.9994}{2.0} \right)}
\]

(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

\[
T_{ox} = T_o - T_a
\]  

\[
C = \left( \frac{W_a}{f_a} \right) \left( \frac{15.9994 N_o}{T_{ox}} \right)
\]

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 diagramatically 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.

ALPHA FACTORS

FINAL JCL CARDS AND COUNTING DATA

PARAMETER CARDS AND COUNT DATA

JCL CARD PROCEEDING DATA

PROGRAM RABBIT

JOB CARD AND JCL CARDS

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

<table>
<thead>
<tr>
<th>Matrix Number</th>
<th>Oxide or Element</th>
<th>Valence</th>
<th>Matrix Number</th>
<th>Oxide or Element</th>
<th>Valence</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O</td>
<td>2</td>
<td>19</td>
<td>CuO</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>CO$_2$</td>
<td>2</td>
<td>20</td>
<td>ZnO</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>F</td>
<td>1</td>
<td>21</td>
<td>Rb$_2$O</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>Na$_2$O</td>
<td>1</td>
<td>22</td>
<td>SrO</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>MgO</td>
<td>2</td>
<td>23</td>
<td>Y$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>Al$_2$O$_3$</td>
<td>3</td>
<td>24</td>
<td>ZrO$_2$</td>
<td>4</td>
</tr>
<tr>
<td>7</td>
<td>SiO$_2$</td>
<td>4</td>
<td>25</td>
<td>BaO</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>P$_2$O$_5$</td>
<td>5</td>
<td>26</td>
<td>La$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>9</td>
<td>SO$_3$</td>
<td>2</td>
<td>27</td>
<td>Ce$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>10</td>
<td>Cl</td>
<td>1</td>
<td>28</td>
<td>Pr$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>11</td>
<td>K$_2$O</td>
<td>1</td>
<td>29</td>
<td>Nd$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>12</td>
<td>CaO</td>
<td>2</td>
<td>30</td>
<td>Sm$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>13</td>
<td>TiO$_2$</td>
<td>4</td>
<td>31</td>
<td>Gd$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>14</td>
<td>Cr$_2$O$_3$</td>
<td>3</td>
<td>32</td>
<td>Dy$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>15</td>
<td>MnO</td>
<td>2</td>
<td>33</td>
<td>Er$_2$O$_3$</td>
<td>3</td>
</tr>
<tr>
<td>16</td>
<td>FeO</td>
<td>2</td>
<td>34</td>
<td>HfO$_2$</td>
<td>4</td>
</tr>
<tr>
<td>17</td>
<td>CoO</td>
<td>2</td>
<td>35</td>
<td>ThO$_2$</td>
<td>4</td>
</tr>
<tr>
<td>18</td>
<td>NiO</td>
<td>2</td>
<td>36</td>
<td>UO$_2$</td>
<td>4</td>
</tr>
</tbody>
</table>
PARAMETER CARD FORMATS

<table>
<thead>
<tr>
<th>Columns</th>
<th>Name</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-80</td>
<td>LABEL</td>
<td>20A4</td>
<td>Title, any characters may be used</td>
</tr>
<tr>
<td>Card 2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-2</td>
<td>L</td>
<td>I2</td>
<td>Number of standards plus backgrounds, maximum = 20</td>
</tr>
<tr>
<td>3-4</td>
<td>M</td>
<td>I2</td>
<td>Number of elements to be analyzed, maximum = 11</td>
</tr>
<tr>
<td>5-7</td>
<td>N</td>
<td>I3</td>
<td>Number of unknowns to be analyzed, maximum = 150</td>
</tr>
<tr>
<td>8-11</td>
<td>OX</td>
<td>F4.1</td>
<td>Number of oxygens/unit cell (for example, 8.0 for feldspars); use 1.0 if option is ignored</td>
</tr>
<tr>
<td>12-13</td>
<td>MSTD</td>
<td>I2</td>
<td>Number of standard elements (for beta-factor calculations); maximum = 11</td>
</tr>
<tr>
<td>14-15</td>
<td>NORM(1)</td>
<td>I2</td>
<td>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</td>
</tr>
<tr>
<td>15-17</td>
<td>NORM(2)</td>
<td>I2</td>
<td>Second element to be normalized for ternary plot</td>
</tr>
<tr>
<td>18-19</td>
<td>NORM(3)</td>
<td>I2</td>
<td>Third element to be normalized for ternary plot</td>
</tr>
<tr>
<td>20-21</td>
<td>ITAB</td>
<td>I2</td>
<td>Option to print analyses in tabular form; blank means no, 1 means yes</td>
</tr>
<tr>
<td>Card 3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-8</td>
<td>ROW(1),ATWT(1)</td>
<td>A2,F6.3</td>
<td>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</td>
</tr>
<tr>
<td>Columns</td>
<td>Name</td>
<td>Format</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>---------------</td>
<td>----------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>9-16,...,</td>
<td>ROW(2),ATWT(2), A2,F6.3</td>
<td></td>
<td>Second channel - tenth channel</td>
</tr>
<tr>
<td>73-80</td>
<td>...ROW(10),ATWT(10)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Card 4</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-8</td>
<td>ROW(11),ATWT(11) A2,F6.3</td>
<td></td>
<td>Eleventh channel; remove this card if 10 or less elements are analyzed</td>
</tr>
<tr>
<td><strong>Card 5</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-2</td>
<td>MFLAG(1) I2</td>
<td></td>
<td>Bence-Albee matrix number (from Table 1); numbers must be in same order as</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>data are taken from microprobe. There must be as many matrix numbers as</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>standard elements (item 5, card 2)</td>
</tr>
<tr>
<td>3-4,...,</td>
<td>MFLAG(2),... I2</td>
<td></td>
<td>Second matrix number - eleventh matrix number</td>
</tr>
<tr>
<td>21-22</td>
<td>MFLAG(11)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Card 6</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-2</td>
<td>VAL(1) I2</td>
<td></td>
<td>Valences (from Table 1); must be in same order as data are taken from</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>microprobe</td>
</tr>
<tr>
<td>3-4,...,</td>
<td>VAL(2),... I2</td>
<td></td>
<td>Second valence - eleventh valence</td>
</tr>
<tr>
<td>21-22</td>
<td>VAL(11)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Card 7</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-16</td>
<td>OXID2(1),OXID1(1) A8,A8</td>
<td></td>
<td>Oxide and element headings to be used for table (for example; FEO FE );</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>must be in same order as data are taken from microprobe; last pair of</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>headings must read TOTAL TOTAL; maximum number of heading pairs = 12;</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>remove cards 7-9 if ITAB = 0 (item 9, card 2)</td>
</tr>
<tr>
<td>17-32,...,</td>
<td>OXID2(2),OXID1(2), A8,A8</td>
<td></td>
<td>Second pair - fifth pair of headings</td>
</tr>
<tr>
<td>65-80</td>
<td>...OXID2(5),OXID1(5)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Columns</td>
<td>Name</td>
<td>Format</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>------</td>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>Card 8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-16,...,</td>
<td>OXID2(6),OXID1(6),</td>
<td>A8,A8</td>
<td>Sixth pair – tenth pair of headings</td>
</tr>
<tr>
<td>65-80</td>
<td>..,OXID2(10),OXID1(10)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card 9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-16,</td>
<td>OXID2(11),OXID1(11)</td>
<td>A8,A8</td>
<td>Eleventh and twelfth pairs of headings</td>
</tr>
<tr>
<td>17-32</td>
<td>OXID2(12),OXID1(12)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**STANDARD CARD FORMATS**

**Card 1**

<table>
<thead>
<tr>
<th>Columns</th>
<th>Name</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-52</td>
<td>HEAD</td>
<td>A52</td>
<td>Title of standard or background; any characters may be used</td>
</tr>
<tr>
<td>53-54</td>
<td>Ml(J,1)</td>
<td>I2</td>
<td>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</td>
</tr>
<tr>
<td>55-56,...,</td>
<td>Ml(J,2),...,</td>
<td>I2</td>
<td>Flags for second – eleventh channels</td>
</tr>
<tr>
<td>57-58</td>
<td>Ml(J,11)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Card 2**

<table>
<thead>
<tr>
<th>Columns</th>
<th>Name</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-6</td>
<td>WT(J,1)</td>
<td>F6.3</td>
<td>Oxide weight-percent of element in first channel</td>
</tr>
<tr>
<td>7-12,...,</td>
<td>WT(J,2),...</td>
<td>F6.3</td>
<td>Second – eleventh channels</td>
</tr>
<tr>
<td>61-66</td>
<td>WT(J,11)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Columns</td>
<td>Name</td>
<td>Format</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>------------------</td>
<td>--------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>Card 3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-6</td>
<td>DATA(NUM,1)</td>
<td>I6</td>
<td>Count data for first channel</td>
</tr>
<tr>
<td>7-8</td>
<td></td>
<td></td>
<td>Blank</td>
</tr>
<tr>
<td>9-14</td>
<td>DATA(NUM,2)</td>
<td>I6</td>
<td>Count data for second channel</td>
</tr>
<tr>
<td>15-16</td>
<td></td>
<td></td>
<td>Blank</td>
</tr>
<tr>
<td>17-22</td>
<td>DATA(NUM,3)</td>
<td>I6</td>
<td>Count data for third channel</td>
</tr>
<tr>
<td>23-24</td>
<td></td>
<td></td>
<td>Blank</td>
</tr>
<tr>
<td>25-30</td>
<td>JTTIME</td>
<td>I6</td>
<td>Counting interval (in $10^{-3}$ sec)</td>
</tr>
<tr>
<td>31-32</td>
<td></td>
<td></td>
<td>Blank</td>
</tr>
<tr>
<td>33-38</td>
<td>ITIME</td>
<td>I6</td>
<td>Total beam current energy in counts</td>
</tr>
<tr>
<td>Card 4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-6</td>
<td>DATA(NUM,4)</td>
<td>I6</td>
<td>Count data for fourth channel</td>
</tr>
<tr>
<td>7-8,</td>
<td></td>
<td></td>
<td>Blank</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>57-62</td>
<td>DATA(NUM,11)</td>
<td>I6</td>
<td>Count data for eleventh channel</td>
</tr>
<tr>
<td>63-64</td>
<td></td>
<td></td>
<td>Blank</td>
</tr>
<tr>
<td>65-70</td>
<td>DATA(NUM,12)</td>
<td>I6</td>
<td>Total energy in counts for energy-dispersive system (for deadtime corrections)</td>
</tr>
</tbody>
</table>

Cards 3 and 4 are repeated for each count; maximum = 40 counts

Cards 5 and 6  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

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

RABBIT was conceived after much urging from G. K. Czamanske. C. R. Bacon and Julie M. Donnelly encouraged adoption of empirical corrections. Mel Beeson, C. R. Bacon, and Vic Adams reviewed the manuscript. Sue Kendall kindly typed the manuscript.
REFERENCES


APPENDIX I: PROGRAM LISTING
PROGRAM RABHIT BY FASER E. GOFF IS A FAST, HIGH VOLUME PROGRAM THAT REDUCES ELECTRON MICROPROBE DATA FROM A SCALER COUNTS TO ELEMENTAL COMPOSITIONS IN WEIGHT PERCENT.

THIS IS A HENCE-ALBEE VERSION FOR OXIDES, SILICATES, CARBONATES, SULFATES, AND PHOSPHATES.

OUTPUT CONSISTS OF:
1. AVERAGED COUNTS CORRECTED FOR BACKGROUND, DEADTIME, AND DRIFT,
2. OXIDE WEIGHT PERCENT,
3. BENCE-ALBEE CORRECTED OXIDE PERCENT,
4. STD DEVIATION OF ALL COUNTING STATISTICS,
5. ATOM WT PERCENT,
6. ATOMIC PROPORTIONS (CATIONS/UNIT CELL),
7. NORMALIZED CATIONS FOR TERNARY PLOT.

DIMENSION UKWT(13), UNKNWN(ISO*12), STD(20,12), SLOPE(20*12)(ROW(12), NAME<150,13), HEAD(13), WT(20*12), DATA(40*12), AVb(12), ATWTU2, LABEL(20), KR(12), COUNT(2), WAIT(2), STIHE(20), TIME(150), ATPRO(12), IFF(40*12), SUM(12), DEV(150*12), DV(12), VAL(12), M1(20*1?), BETA(12), SBETA(12), SDEV(20*12), MFLAGU2, NORM(3), ALPHA (36,36), XH(12)

DIMENSION TAB1(150*12), TAB2(150*12), 0X101(12), 0X102(12)

INTEGER DATA*VAL, R

REAL 8 KW, OXID1, OXID2

READ IN BENCE-ALBEE ALPHA FACTORS

DO 4443 J=1,36
READ 4444,(ALPHA(I,J),I=1,9)
READ 4444*(ALPHA(I,J)),I=1,9
READ 4444*(ALPHA(I,J),I=1,9)
READ 4444*(ALPHA(I,J),I=1,9)
4444 FORMAT(6X,9(F6.3,1X))
4443 CONTINUE

READ IN PARAMETERS AND PROBE DATA

501 READ 299, LABEL
299 FORMAT (20A4)
READ 300, L, M, N, OX, MSTO. (NORM(I),I=1,3), ITAB
300 FORMAT (*FA, 212.13.F4.1)
IF (L) 500, 500, 502
502 READ 302, (ROW(I), ATWT(I), I=1, M)
302 FORMAT (12(A2.F6.3))
READ 506, (MFLAG(I), I=1, M)
506 FORMAT (1212)
READ 305, (VAL(I), I=1, M)
305 FORMAT (1212)

MZ-M+1

IF (ITAB) 303, 303, 716
716 READ 701, (0X102(I), OXIOUI), I=1,MZ
701 FORMAT (30A8)
303 PRINT 298, LABEL, L, M, N, MSTO, OX
298 FORMAT (iH1, 20A4, //.5X, 9HNO. STDS«, I2*5A, 9HNO. ELEMs*I2, 5X, 113HNO. UNKNOWNS-, 13.5X, 13HNO. STD ELEM», I2*5X, 12HNO. OXYGENS', 2F4.1, //)
PRINT 297
READ STANDARDS AND BACKGROUNDS

READ 301*(WT(J,M)).I=1.MSTD)

C COMPUTE STANDARD BETA FACTORS

IF (KK> 419.00 422.1»1»MSTD)
IF (M(J,M)-1) 422»4?2»423
JFLAG » MFLAG(M)
SBETA(M)» WT(J,M)   ALPHA(JFLAG*IFLAG) * SBETA(M)
TOTWT, TOTWT * WT(J,M)
424 CONTINUE
S8ETA(M)» SBETA(M)/TOTWT
422 CONTINUE

C AVERAGING SECTION

104 I=!*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,I)
110 FORMAT (I6«4(2X«I6)>)
READ 111.(DATA(NUM.I).I=4.11).R
111 FORMAT (I6«8(2X«I6)>)
IF (DATA(NUM.I) 500*112.113
113 00 114 1-1.12
AVE(I)»AVE(I)*DATA(NUM.I)
114 CONTINUE
S»S*1TIME
T»T*JTIME
GO TO 109
112 NUM»NUM-1
115 CONTINUE
AVE(I)=AVE(I)/NUM
115 CONTINUE
T»T/NUM
ENERGY=ENERGY/NUM
S=(S/NUM)*0.001
C COMPUTE STANDARD DEVIATION OF COUNTS

IF (NUM-1) 63t63.62
 62 00 69 K*1.NUM
 00 68 I«1.M
DIFF(NUM.I)«<AVE(I>-r)ATA(NUM.n) (AVE(I>-DATA(NUM.I))
  SUM(I)*SUM(I)*OIFF(NUMtI)
68 CONTINUE
69 CONTINUE
00 67 I«1.M
  SUM(I)*SORT(SUM(I)/(NUM-1))
67 CONTINUE
GO TO 61
60 00 66 I«1»M
  SUM(I)« 0.0
66 CONTINUE
61 IF (Tl> 38t38t39
 38 THOLD-T
39 Tl«Tl*l
C APPLY OEAOTIME CORRECTION TO ENERGY DISPFUSIVE SYSTEM
00 160 I»1.M
IF (1-3) 160tl60tl61
161 X1«ENERGY/S
165 X2»(ENERGY/S)»EXP<-X1«7.5E-05)
X3»ABS<X2-X1)
X4»X2»1.0£-05
162 IF <X3«X4) I62.163tl63
163 X1-X2
GO TO 165
162 AVE(I)"AVE(I) ((ENERGY/S)/X2)
160 CONTINUE
IF (KK) 20t20t21 ,
C PRINT STANDARD INFORMATION
20 DO 32 I«ltM
IF (MKJtD) 30*30t31
31 STO (JtD»AVE(I>
50EVI(JtI)B(SUH(I)*WT(JtI))/STD(J*I)
GO TO 32
30 STO(J.I). 0.0
50EVI(J.I). 0.0
32 CONTINUE
STIME(J)"T«.THOLD
IF (KK) 46t47t47
46 PRINT 45
45 FORMAT (iHOtSXtSHSTART)
GO TO 48
47 PRINT 49
49 FORMAT (1H0.5X.6HFINISH)
48 PRINT 25»HEAO.STIME(J)
25 FORMAT (1HO«/*5X»13A4*5HTIME**F9.3*/)
PRINT 220*(ROW(I)*I«1*MSTO)
220 FORMAT (In *17X*12(A4*6X))
PRINT 28*(STO(J»I»I*1.M)
28 FORMAT (1H0.11HAVE COUNTSs.12(F10.3))
PRINT 26t(WT(J*I)*I*1fMSTO)
26 FORMAT (1H .11HWT PERCENT*.i2(F10.3))
PRINT 65»(SOEV(J,I)»I*1.M)
65 FORMAT (1H0, 1H4, 1H0, 1H6, 1H0, 1H4, 1H0, 3X, 1H6, 1H0, 1H4, 1H0, 3X, 1H12, 1H0)
5 CONTINUE
C
C READ IN UNKNOWN DATA
C
36 FORMAT (13A4)
GO TO 104
21
00 00 41 Irl.M
UNKNOWN(J,I)*AVE(I)
OEV(J,I) = SUM(I)
41 CONTINUE
TIME (J) = T-THOLD
42 CONTINUE
KKO
M2 » L
L = L/2
PRINT 8
8 FORMAT (1H1*21HSTANDARD BETA FACTORS/)
PRINT 4t (SBETAU) .IM.MSTD)
4 FORMAT (1H0.11H BETA FACTORS,12(F10.3),////)
C
C CALCULATE DRIFT IN STOS BY LINEAR EQUATIONS
C
00 215 J = L
00 216 I » 1.M
IF (STO(J)) 217 » 217*218 00
217 SLOPE(J,I) = (STO(J,L) - STD(J,I)) / (STIME(J,L) - STIME(J))
GO TO 216
218 SLOPE(J,I) = O.O
216 CONTINUE
21S CONTINUE
C
C INTERPOLATE BETWEEN STO AND BKGO VALUE. CALCULATE RAW COMPOSITIONS
C
PHINT 257
257 FORMAT (1HO»31HUNKNOWN COUNTS AND COMPOSITIONS/)
00 280 K = 1.N
00 265 I = 1.M
N2al
00 266 J = L
IF (SLOPE(J,I)) 267 » 266t267
267 COUNT(N2) = SLOPE(J,L) * TIME(J) - SLOPE(J,I) * STIME(J)
WAIT(N2) = WT(JI)
N2 = N2*1
266 CONTINUE
SLOP = (COUNT(2) - COUNT(1)) / (WAIT(2) - WAIT(1))
UKWT(I) = ((UNKNOWN(K,I) - COUNT(1) * SLOPE(WAIT(1))) / SLOP)
IF (UKWT(I)) 3.265 » 265
3 UKWT(I) = 0.0
265 CONTINUE
C
C COMPUTE BENCE-ALBEE CORRECTED COMPOSITIONS
C
TOTKR = 0.0
3 CONTINUE
4 FORMAT (1H4, 1H16, 1H FACTOR=I12,10.3)
PRINT 4 (SBETAU) .IM.MSTD)
0 FORMAT (1H4, 1H16, 1H FACTOR=I12,10.3)
PRINT 8
8 FORMAT (1H1*21HSTANDARD BETA FACTORS/)
PRINT 4*(SBETAU) .IM.MSTD)
4 FORMAT (1H0.11H BETA FACTORS,12(F10.3),////)
C
C CALCULATE DRIFT IN STOS BY LINEAR EQUATIONS
C
00 14 TIME(J) = T-THOLD
14 CONTINUE
C
C READ IN UNKNOWN DATA
C
5 CONTINUE
65 FORMAT (1H4, 1H16, 1H FACTOR=I12,10.3)
1) 0.44 0.1*1.*
KRU (UKMT/SHETA(I)» XH(I)» KK(I)
TOTKR* KR(I) * TOTKR
440 CONTINUE
FLAG» 0.0
444 0.0 445 1*1»M
BETAU>» 0.0
CONTINUE
J»1,M
JFLAG» MFLAG(J)
I»1.M
IFLAG» MFLAG(I)
BETAU)” KR(I)» ALPHAUFLAG.IFLAG) * 8ETA(J)
CONTINUE
8ETA(J)« 8ETA(J)/TOTK«
CONTINUE
TOTKR»0.0
J»1.M
KR(J>« RETA(J) * XR(J)
TAB!(KfJ)» KR(J)
TOTKRa KR(J) * TOTKR
CONTINUE
TABKK»M*1>» TOTKR
FLAG* FLAG * 1.0
IF (FLAG=2.0) 444«444t446
C
C PRINT ANALYSES
C
268 FORMAT (1H10,T1.3I3X,13A4I2X,(11H TIME»»F9.3)/)
PRINT 258,(ROW(I>tl»l*M>
258 FORMAT (1H0t17Xil2(A4i6X))
PRINT 269i(UNKNWN(Kif).I«liM)
269 FORMAT (lHOtllHAVE COUNTS*.12(F10,3))
PRINT 270*(UKWT(I>ilaliM)
270 FORMAT (1H tllH OXIDE PER»i12(F10.3))
PRINT 292i(BETA(I>tIal*M)
292 FORMAT (1H tllH BETA FACT*i12(F10.3)>)
PRINT 408i(KR(I)tl'ltM)
408 FORMAT (1H tllH B-A CORR.t12(F10.3))
PRINT 272.TOTKR
272 FORMAT (1H .11HTOT WT PER«iF10.3)
C
C COMPUTE TOTAL STO DEVIATION W/ PARTIAL DIFFERENTIALS
C
64 JaliL
641 IMtM
IF (MKJiI)-l) 642*643,644
642 GO TO 641
643 DV(I)» <(MT(JtI) * OEV(K,I))/STO(JiI))«»?.0 * (( UNKNWN(KiI)
1   WT(J,I)   SDEV(J.D) /(STO(J»I)   STO(Jtl))) »»2.0
OV(I)« SQRT(DV(I»
641 CONTINUE
64 CONTINUE
PRINT 271,( nV(D,1=1.M)
271 FORMAT (1H0.11H STO OEV«,12(FlO.3))
C
C NORMALIZE THREE ELEMENTS FOR TERNARY DIAGRAMS
C
IF (NORM(1)) 460*464
464 TNORM = 0.0, CO
DO 460 INORM = NORM(1)
460 CONTINUE
IF (TNORM) 280*465
465 DO 461 INORM = NORM(1)
461 CONTINUE
PRINT 462*(UKWT(NORM(I)), I=1, NORM(3))
462 FORMAT (52HNORMALIZED ATOM RATIOS FOR TERNARY PLOT OF ELEMENTS)
280 CONTINUE
IF (ITAB) 720*721
721 MG = 0
MF = -1
KX = N
710 IF (KX-12) 708*708.709
708 MF = MF + 12
MG = MG + 12
709 GO TO 711
709 MF = MF + 12
MG = MG + 12
711 PRINT 700
700 FORMAT (//)
PRINT 718*(NAME(K, JJ), JJ=1, 2) K, MF, MG)
718 FORMAT (12(2X*2A4))
CONTINUE

FORMAT (1HO./.1X.26HCATIONS/UNIT CELLI OXYGFN*.F4.1t//)

PRINT 713. OXI02<TAB2<K.I)tK»MFtMG)

IF (KX-12) 501.501.

KX= KX-12
FORMAT (1HO./.1X.26HCATIONS/UNIT CELLI OXYGFN*.F4.1t//)

PRINT 713. OXI02<TAB2<K.I)tK»MFtMG)

DO 715 I=1,4

714 FORMAT (1HO./.1X.26HCATIONS/UNIT CELLI OXYGFN*.F4.1t//)

PRINT 714. OXI02<TAB2<K.I)tK»MFtMG)

CONTINUE

STOP
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.
<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

HEDCNBERGITE

2.92 24

AMPHIdULF 52-4

TOTAL

TOTAL

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

FECa 99+ FeO 92+ MgO 11+ Ca 7+ Al 4+ Ti 2+ O 3+ Si 22+ Sr 2+
APPENDIX III: SAMPLE OUTPUT LISTING
PYROXENES OF 15 DEC 751 15 KV .03 MA SECOND BATCH

NO. STUNS 4 NO. ELEMA 7 NO. UNKNOWNS 5

STANDARD COUNTS AND COMPOSITIONS

START

NO. STU ELEMS 9

OXYGENS 6.0

DIOPSIDE CPX-1

FE AVE COUNTS 0.0
NT PERCENT 2.920
STD DEV 0.0

CA 1161.250
24.560
0.093

Mg 7596.398
16.930
0.358

Si 6253.934
53.930
0.465

TIMF AL 0.0
0.660
0.0

AMPHIBOLE ZP 24

START

BACKGROUNDS OFF AL2O3. SIO2,

AVE COUNTS
NT PERCENT
STD DEV

FINISH

OIOPS10E

AVE COUNTS
NT PERCENT

BACKGROUNDS OFF AL2O3. SIO2. AND CPX-1

FINISH

START

MEChEBRITE C-9

START

DIOPSIDE CPX-1

STANDARD COUNTS AND COMPOSITIONS

NO. STUNS 4 NO. ELEMA 7 NO. UNKNOWNS 5 NO. SIU ELEMA 9
NO. OXYGENS 6.0

PARAXENES OF 15 DEC 751 IS KY 103 MA SECOND RACH
<table>
<thead>
<tr>
<th>Name</th>
<th>Count</th>
<th>Weight</th>
<th>Std Dev</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>50.000</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Ca</td>
<td>120.000</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Mg</td>
<td>60.000</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Si</td>
<td>627.501</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Al</td>
<td>936.688</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Mn</td>
<td>167.714</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Ti</td>
<td>341.132</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>Na</td>
<td>527.721</td>
<td>3.080</td>
<td>0.171</td>
</tr>
<tr>
<td>K</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**References:**
- Background of Al2O3 SiO2 MgO CaO.
### Known Counts and Compositions

<table>
<thead>
<tr>
<th>Element</th>
<th>Count</th>
<th>Oxide Percentage</th>
<th>Beta Factor</th>
<th>B-A Correction</th>
<th>Total Weight Percentage</th>
<th>Standard Deviation</th>
<th>Atomic Percentage</th>
<th>Atomic Proportion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>3456.75</td>
<td>41.13%</td>
<td>1.114</td>
<td>1.057</td>
<td>39.74%</td>
<td>0.183</td>
<td>0.436</td>
<td></td>
</tr>
<tr>
<td>Ca</td>
<td>8763.75</td>
<td>19.23%</td>
<td>1.070</td>
<td>1.114</td>
<td>18.45%</td>
<td>0.316</td>
<td>0.735</td>
<td></td>
</tr>
<tr>
<td>Mg</td>
<td>5352.75</td>
<td>11.91%</td>
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### Standard Beta Factors

| Beta Factor | 1.150 | 1.170 | 1.090 | 1.110 | 1.130 | 1.050 | 1.110 |

### Additional Data

- **CASI Begin Analyses of Second Group of Proxemics Time = 654.438**
- **CASI Begin Analyses of Second Group of Proxemics Time = 694.389**
- **CASI Begin Analyses of Second Group of Proxemics Time = 704.988**
- **CASI Begin Analyses of Second Group of Proxemics Time = 784.988**
- **CASI Begin Analyses of Second Group of Proxemics Time = 812.988**
- **CASI Begin Analyses of Second Group of Proxemics Time = 834.988**
- **CASI Begin Analyses of Second Group of Proxemics Time = 864.988**
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