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AN APL LANGUAGE COMPUTER PROGRAM FOR USE IN ELECTRON MICROPROBE ANALYSIS

By

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and

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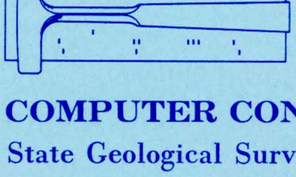

COMPUTER CONTRIBUTION 45

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Editor's Remarks

"An APL language computer program for use in electron microprobe analysis", by D.G.W. Smith and M.C. Tomlinson is our first APL program. In the past, programs have been published in several languages including BALGOL, ALGOL, FORTRAN II, and FORTRAN IV. APL is a very versatile language and will undoubtedly be used much by scientists. The following table indicates in which language programs are available from the Geological Survey. Several programs are available in different versions.

Language	Geological Survey Publication
BALGOL	SDP3*, SDP9*, SDP24, B171, CC1*
ALGOL	SDP23, CC2, CC8
FORTRAN II	SDP4*, SDP12, SDP13, SDP14, SDP26, SDP28, CC4, CC10, CC15, CC19, CC20, CC37, CC38
FORTRAN IV	SDP12, SDP23, B170-3, B171, CC2, CC3, CC5, CC6, CC9, CC11, CC13, CC14, CC15, CC16, CC17, CC20, CC21, CC23, CC24, CC25, CC26, CC27, CC28, CC29, CC30, CC31, CC32, CC33, CC34, CC35, CC36, CC39, CC41, CC42, CC43, CC44, CC45
APL	CC45

*out of print; SDP=Special Distribution Publications; CC=Computer Contributions; B=Bulletins.

Computer Contribution

2.	A generalized two-dimensional regression procedure, by J.R. Dempsey, 1966	$0.50
3.	FORTRAN IV and MAP program for computation and plotting of trend surfaces for degrees 1 through 6, by Mont O'Leary, R.H. Lippert, and O.T. Spitz, 1966	$0.75
4.	FORTRAN II program for multivariate discriminant analysis using an IBM 1620 computer, by J.C. Davis and R.J. Sampson, 1966	$0.50
5.	FORTRAN IV program using double Fourier series for surface fitting of irregularly spaced data, by W.R. James, 1966	$0.75
6.	FORTRAN IV program for estimation of cladistic relationships using the IBM 7040, by R.L. Bartcher, 1966	$1.00
7.	Computer applications in the earth sciences: Colloquium on classification procedures, edited by D.F. Merriam, 1966	$1.00
8.	Prediction of the performance of a solution gas drive reservoir by Muskat's equation, by Apolonio Baca, 1967	$1.00
9.	FORTRAN IV program for mathematical simulation of marine sedimentation with IBM 7040 or 7094 computers, by J.W. Harbaugh and W.J. Wahlstedt, 1967	$1.00
10.	Three-dimensional response surface program in FORTRAN II for the IBM 1620 computer, by R.J. Sampson and J.C. Davis, 1967	$0.75
11.	FORTRAN IV program for vector trend analyses of directional data, by W.T. Fox, 1967	$1.00
12.	Computer applications in the earth sciences: Colloquium on trend analysis, edited by D.F. Merriam and N.C. Cocke, 1967	$1.00

(continued on inside back cover)

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INTRODUCTION

The intensities of characteristic x-ray lines excited during an electron probe analysis are only approximately proportional to the concentrations of the elements present within the sample. It is well known that to obtain quantitative analyses various corrections must be applied. For a summary of the corrections the reader is referred to the excellent review articles of Keil (1967), Long (1967) and Sweatman and Long (1969).

PROBEDATA is an APL language program for correcting raw x-ray intensity data from an electron microprobe for background, dead-time, atomic number, absorption and characteristic fluorescence effects. The program can be used in the analysis of any element with atomic number in excess of ten at any integral operating voltages up to 35KV and will accomodate data for the specimen and several different standards composed of up to 20 elements. (At the present time it is impractical to apply corrections to apparent concentrations of elements with atomic numbers of 10 or less, because of the paucity of data on mass absorption coefficients at long wavelengths). Facilities also are provided for adjusting the composition of the material analyzed on some basis such as the structural formula of a mineral, or perhaps the assumed anion content on the basis of the concentrations of other elements present. This program was written primarily to deal with analyses of geological materials, but will be applicable to analyses of other materials such as ceramic and metallurgical specimens, without modification to the main program or subroutines. It was designed for use with an ARL "EMX" microprobe, but with minor modifications can be used with any of the electron probes currently on the market which have a normally incident electron beam. Fairly substantial modifications to the absorption and fluorescence corrections and different R values in the atomic number correction would be required for use with instruments such as those manufactured by AEI and MAC which have oblique electron incidence.

In writing the program, emphasis has been placed on making it suitable for as wide a range of materials as possible, rather than on providing sophisticated facilities for the input of data in variable amounts and variable form. It is considered more convenient to perform simple preliminary procedures, such as the averaging of data, on an electronic desk calculator although limited optional facilities for this have been provided. Thus the program is particularly well suited for use with a wide range of different samples rather than a large number of similar samples run in one batch. However, facilities have been included whereby a large group of samples run against one set of standards may be corrected at one time by activating an optional loop.

For a description of APL, the reader is referred to the IBM user's manual (Falkoff and Iverson, 1968).

Acknowledgments.- We are grateful to Dr. J. Rucklidge of the University of Toronto, Dr. S.J.B. Reed of the Department of Mineralogy, British Museum (Natural History), and Mr. G. Gabel of the Department of Computing Science, University of Alberta, for valuable advice in the preparation of this program. One of us (D.G.W.S.) is pleased to acknowledge financial support from the National Research Council of Canada for this work.

GENERAL FORM OF PROGRAM

The mainline program is *PROBEDATA* (Fig. 1). This calls the subroutine *READATA* to average readings for peaks and backgrounds on the specimen and standard(s) and then make corrections for background and dead-time (the latter being an optional facility). The apparent concentrations then are printed out, together with the corrected counts for the standard and specimen. Once *READATA* has been completed, *PROBEDATA* goes on to make corrections for atomic number and absorption effects and then calls *FLC* to compute the fluorescence corrections. The last three corrections are in the form of a loop, and the program will emerge from this loop only when there is satisfactory consistency between the last two sets of corrected values for the element concentration being corrected. The consistency demanded of the values may be adjusted by the user. Once this iterative procedure has been completed satisfactorily for one element the program continues with the next element using the corrected concentrations of the previous elements. If the corrections are large so that the corrected concentrations are outside the limits of consistency demanded by the user, the program then returns to the first element to recompute that correction. This process is continued until all analyzed elements have been corrected. It will next print out the corrected concentrations followed by the atomic number, absorption and fluorescence corrections. At the choice of the user it will then call for data for the next specimen (and/or new

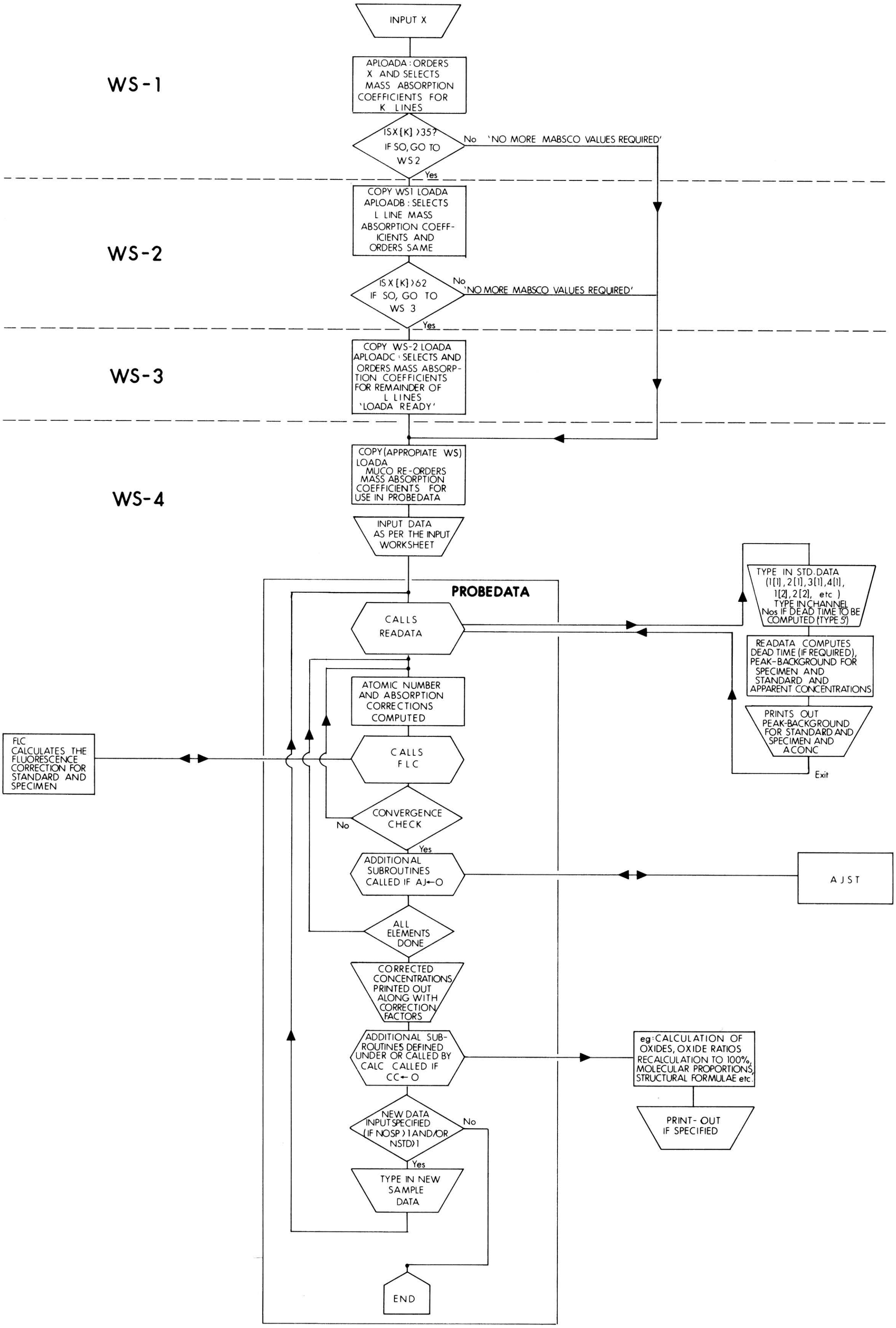

Figure 1.- Schematic flow-sheet for *PROBEDATA*

intensity data for the same group of standards) - or alternatively terminate its operation.

In addition to the subroutines mentioned above, the main workspace also must contain the subroutine *MUCO* which orders the mass absorption coefficients (copied previously from storage workspaces) into the form required by *PROBEDATA* and subroutines. The short subroutine *R←N RND X* is used to round-off concentrations, etc. The desired number of decimal places is substituted for *N* whenever the subroutine appears in the program *(PROBEDATA [41], [43], [45], [47]; READATA [33], [35])*. The values of *N* listed in the program as reproduced here may be changed by the user. *AJST* is a variable subroutine defined in name only and intended for use by the operator in performing adjustments to the concentrations of assumed elements, for example, after each iteration of the correction procedures. Some examples of the definition and use of *AJST* are given in Optional and Special Facilities. *CALC* is another similar variable subroutine, but in this situation is intended for use after all corrections have been made, so that, for example, the structural formula of a mineral may be calculated from the corrected output from the main program.

A large number of mass absorption coefficients are required if the program is to be able to deal with a wide range of different materials, without the necessity for the operator to look up and type in required values. It is necessary therefore to keep the coefficients in three storage workspaces. They may be combined by the programs *APLOADA*, *APLOADB*, and *APLOADC* and copied into the main workspace containing *PROBEDATA*, etc., ready for ordering by *MUCO* for subsequent use. For this purpose only the atomic numbers of elements present in specimen and standard(s) need be specified.

SUMMARY OF CORRECTIONS APPLIED

PROBEDATA uses the formulae and data of Duncumb and Reed (1968) to accomplish the atomic number correction (Table 1). Thus the stopping power for a specimen or standard is computed as $\overline{S} = \Sigma S x C$, where S and C are the stopping power and mass concentration respectively for each of the elements present. For each element, S is obtained from the expression:

$$S = \text{const.} \times (Z/A \times 1/E \times \ln(1.166 \times E/J)),$$

where Z = atomic number of an element present in the material,

A = atomic weight of the same element,

$E = 1/2(E_o + E_k)$,

E_o = operating voltage at which element being determined was excited (in eV),

E_k = critical excitation voltage of the element determined (in eV), and

J = mean ionization potential of the element for which S is calculated.

J values for a particular element are given by Duncumb and Reed (1968) and have been stored for use in the program under the same variable name (Table 2). The other part of the atomic number correction, R, the back-scatter coefficient, changes with average atomic number and overvoltage (the ratio of operating voltage to critical excitation voltage for the particular line being used in the determination of the element being analyzed). The table of R values given by Duncumb and Reed (1968) is used to obtain the values required in the correction procedure by extrapolation to the precise atomic number and overvoltage applicable, linear variation between given values being assumed (Table 3). Thus once the values of S/R have been computed for the specimen and standard, the apparent concentrations may be multiplied by the factor $(S/R)_{sp}/(S/R)_{st}$ to give the first corrected concentrations (sp and st refer to specimen and standard, respectively). "const." and "1/E" cancel out at this point and thus need not be computed.

At the same time as the atomic number correction is computed, the absorption correction also is determined and applied to the apparent concentrations before the subroutine *FLC* is called. The formula used for the absorption correction is from Philibert (1963) as modified subsequently by Heinrich (1967). This seems to be preferable to the Duncumb and Shields (1966) modification (see Duncumb, Shields-Mason, and Da Casa, 1968; and Sweatman and Long, 1969). The formula is

$$F(\chi) = \frac{1 + h}{(1 + \chi/\sigma)(1 + h(1 + \chi/\sigma))},$$

where $\chi = (\mu/\rho) \operatorname{cosec} \theta$,

μ/ρ = average mass absorption coefficient of specimen for the wavelength of the analysis line,

θ = take-off angle of the x-rays,

$\sigma = (4.5 \times 10^5)/(E_o^{1.65} - E_c^{1.65})$,

E_o = operating voltage in KeV at which element being determined was excited,

E_c = critical excitation voltage of element being determined, in KeV,

$h = 1.2 \times \overline{(A/Z^2)}$, and

$\overline{(A/Z^2)}$ = average value for the specimen of atomic weight divided by the square of the atomic number.

The mass absorption coefficients used are those computed by Heinrich (1966) by interpolation of the most reliable of the experimental data. An exception however, is μ_{Na}^{Na} for which the value of 500 recommended by Smith (1965) is used.

Table 1.- Fluorescence data of Reed (1965).

Atomic Number	Equivalent Atomic No.	Limiting atomic number for excitation by				J(A) for excitation by	
		K_{α_1}	K_{β_1}	L_{α_1}	L_{β_1}	K	L
11	11	12	12	31	31	0.008	0.006
12	12	13	13	34	33	0.011	0.009
13	13	14	14	36	36	0.015	0.011
14	14	15	15	39	38	0.020	0.015
15	15	16	16	41	41	0.025	0.019
16	16	17	17	44	43	0.032	0.024
17	17	18	18	46	45	0.039	0.030
18	18	00	00	00	00	0.000	0.000
19	19	20	20	52	50	0.056	0.045
20	20	21	21	55	53	0.067	0.056
21	21	22	22	57	55	0.078	0.071
22	22	24	23	59	57	0.102	0.079
23	23	25	24	62	59	0.115	0.086
24	24	26	25	64	62	0.132	0.096
25	25	27	26	67	64	0.145	0.111
26	26	28	27	69	66	0.155	0.123
27	27	29	28	72	68	0.170	0.140
28	28	30	29	74	70	0.180	0.155
29	29	31	30	77	72	0.200	0.175
30	30	32	31	79	74	0.210	0.190
31	11.1	33	32	82	77	0.220	0.210
32	11.5	34	33	85	79	0.240	0.230
33	12.1	35	34	87	81	0.250	0.240
34	12.5	37	35	90	83	0.260	0.260
35	13.0	14	14	36	36	0.009	0.006
36	00.0	00	00	00	00	0.000	0.000
37	13.8	15	14	39	38	0.011	0.007
38	14.3	15	15	40	39	0.011	0.008
39	14.9	16	15	41	40	0.014	0.009
40	15.2	16	16	42	41	0.014	0.010
41	15.7	17	16	43	42	0.018	0.011
42	16.2	17	17	44	43	0.018	0.012
43	00.0	00	00	00	00	0.000	0.000
44	17.0	18	18	46	46	0.022	0.015
45	17.5	19	18	48	47	0.027	0.017
46	18.0	19	18	49	48	0.027	0.019
47	18.4	20	19	50	49	0.032	0.020
48	18.8	20	19	51	50	0.032	0.022
49	19.3	21	20	52	51	0.038	0.023
50	19.7	21	20	53	52	0.038	0.025
51	20.2	22	21	55	53	0.044	0.028
52	20.7	22	21	56	54	0.044	0.030
53	21.1	23	22	57	55	0.050	0.033
54	00.0	00	00	00	00	0.000	0.000
55	22.1	24	23	59	57	0.057	0.037
56	22.6	24	23	61	58	0.057	0.041
57	23.1	25	24	62	59	0.065	0.044
58	23.5	25	24	63	61	0.065	0.046
59	23.9	26	25	64	62	0.072	0.049
60	24.4	26	25	65	63	0.072	0.051
61	00.0	00	00	00	00	0.000	0.000
62	25.3	27	26	67	65	0.080	0.057
63	25.7	28	26	69	66	0.087	0.062
64	26.2	28	27	70	67	0.087	0.066
65	26.7	29	27	71	67	0.095	0.069
66	27.2	29	28	72	69	0.095	0.072
67	27.6	30	28	73	69	0.103	0.075
68	28.1	30	29	74	70	0.103	0.078
69	28.5	31	29	75	71	0.110	0.081
70	28.9	31	30	77	72	0.110	0.088
71	29.4	31	30	78	73	0.110	0.092
72	29.8	32	30	79	74	0.120	0.095
73	30.3	32	31	80	75	0.120	0.099
74	30.7	33	31	81	76	0.125	0.102
75	31.2	33	32	82	77	0.125	0.106
76	31.7	34	32	84	78	0.130	0.110
77	32.2	34	33	85	79	0.130	0.120
78	32.6	35	33	86	80	0.140	0.120
79	33.1	36	34	87	81	0.140	0.120
80	33.5	36	34	88	82	0.140	0.130
81	34.0	37	35	89	83	0.150	0.130
82	34.5	37	35	90	84	0.150	0.140
83	35.0	38	36	92	85	0.160	0.140
84	35.4	38	36	93	86	0.160	0.145
85	35.8	39	36	94	87	0.164	0.148
86	36.3	39	37	95	88	0.167	0.152
87	36.8	39	37	96	89	0.170	0.156
88	37.2	40	38	97	90	0.174	0.160
89	37.7	41	38	98	91	0.177	0.164
90	38.2	41	39	99	92	0.181	0.168
91	38.6	42	39	100	93	0.185	0.172
92	39.1	42	40	100	94	0.188	0.176

Table 2.- J values for particular elements (from Duncumb and Reed, 1968).

J values arranged in order of increasing atomic number from 1 to 94.

150	150	150	150	150	146	135	127	123	123
126	133	142	154	166	180	194	209	224	239
255	270	286	301	316	332	347	362	377	392
407	422	437	451	466	481	495	510	524	538
553	567	581	595	609	623	637	651	665	679
692	706	720	734	747	761	775	788	802	815
829	843	856	870	883	897	910	923	937	950
964	977	991	1004	1017	1031	1044	1057	1071	1084
1097	1111	1124	1137	1151	1164	1177	1191	1204	1217
1231	1244	1257	1270						

LNCO values arranged in order of increasing operating voltage from 1 to 35 KV.

27500	23000	21500	18500	16500	15000	13500	11800	10650	9600
8700	7850	7100	6450	5900	5350	4850	4450	4075	3725
3450	3200	2950	2725	2550	2375	2200	2075	1950	1820
1700	1600	1515	1425	1340					

XF constants associated with logarithmic equations fitted to Reed's (1965) D function and arranged in order of increasing operating voltage from 1 to 35 KV.

-0.2025	-0.1915	-0.1815	-0.1724	-0.1642	-0.1564	-0.1496	-0.1434	-0.1377	-0.1324
-0.1277	-0.1233	-0.1193	-0.1155	-0.1120	-0.1082	-0.1051	-0.1023	-0.0996	-0.0970
-0.0947	-0.0926	-0.0905	-0.0886	-0.0868	-0.0851	-0.0834	-0.0819	-0.0805	-0.0792
-0.0781	-0.0771	-0.0762	-0.0754	-0.746					

ZL: atomic number of elements corresponding to code number 1-90.

11	12	13	14	15	16	17	19	20	21
22	23	24	25	26	27	28	29	30	31
32	33	34	35	37	38	39	40	41	42
43	44	45	46	47	31	32	33	34	35
37	38	39	40	41	42	44	45	46	47
48	49	50	51	52	53	55	56	57	58
59	60	61	62	63	64	65	66	67	68
69	70	71	72	73	74	75	76	77	78
79	80	81	82	83	84	87	90	91	92
93	94								

Table 3.- Values of backscatter coefficients R as function of overvoltage (1/U) and atomic number (Z).

Z \ 1/U	0.01	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
0.	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
10.	0.934	0.944	0.953	0.961	0.968	0.975	0.981	0.988	0.993	0.997	1.000
20.	0.856	0.873	0.888	0.903	0.917	0.933	0.948	0.963	0.977	0.990	1.000
30.	0.786	0.808	0.828	0.847	0.867	0.888	0.911	0.935	0.959	0.981	1.000
40.	0.735	0.760	0.782	0.804	0.827	0.851	0.878	0.907	0.938	0.970	1.000
50.	0.693	0.718	0.741	0.764	0.789	0.817	0.847	0.881	0.919	0.959	1.000
60.	0.662	0.688	0.713	0.737	0.764	0.793	0.825	0.862	0.904	0.950	1.000
70.	0.635	0.663	0.687	0.713	0.740	0.770	0.805	0.844	0.889	0.941	1.000
80.	0.611	0.639	0.665	0.691	0.718	0.750	0.785	0.826	0.874	0.932	1.000
90.	0.592	0.613	0.639	0.665	0.695	0.730	0.767	0.811	0.862	0.924	1.000
99.	0.578	0.606	0.634	0.661	0.691	0.725	0.763	0.806	0.858	0.921	1.000

The program then checks for fluorescent excitation of the analysis line by any and all of the elements listed as present in the sample (specimen and then standard). When the possibility of fluorescent excitation exists, the corrections are computed according to the method of Reed (1965) which takes into consideration K-K, K-L, L-K, and L-L fluorescence, and is the most comprehensive at present available. Apparent concentrations are multiplied by the factor $1/(1+\gamma)$, where γ is

$$C_B \times J(A) \times D \times \frac{\mu_B^A}{\mu_B} (g(x) + g(y)),$$

in which

C_B = mass concentration of the exciting element "B";

$J(A)$ is a function of the analyzed element "A" tabulated by Reed by atomic number for excitation by K or by L lines;

D is a function of the operating voltage and the difference in atomic number of the exciting and excited elements. It is graphed by Reed for a range of values of atomic number difference; equations have been fitted to the curves for the purpose of this program;

μ_B^A is the mass absorption coefficient of the analyzed element A for radiation from another element B which also is present;

μ_B is the mass absorption coefficient of the specimen for radiation from another element B which also is present;

$g(x)$ is a function of x given by the formula $(\ln(1+x))/x$, where

x = $(\mu A/\mu B) \times \operatorname{cosec} \theta$;

μ_A is the mass absorption coefficient of the specimen for K radiation of the analyzed element A;

θ is the take-off angle of the x-rays;

$g(y)$ is a function of y given by the formula $(\ln(1+y))/y$, where

y = σ/μ and is the electron mass absorption coefficient (i.e. Lenard coefficient) which is tabulated for various accelerating voltages by Philibert (1963) and which has been extrapolated here to cover lower operating voltages - see Table 4.

OPTIONAL AND SPECIAL FACILITIES

A number of optional facilities are available within the program. In general these can be activated by simply setting certain variables to zero before calling *PROBEDATA* . The variables are reset automatically to 1 to make the facility inactive before the program terminates.

AJST (Called if *AJ←0*)

This is a dummy subroutine which can be made to perform various functions during the operation of the program at the end of each iteration of the atomic number, absorption and fluorescence corrections.

Example: It might be desirable to reset an assumed oxygen content for a specimen on the basis of the new, corrected concentrations for the analyzed elements. This could be done as

```
      ∇ AJST
[1]     CONC[NUM+1]← +/(CONCxFAC)-CONC[⍳NUM],
      ∇
```

where *FAC* is a list of oxide conversion factors (specified outside the program), *NUM* is the number of elements analyzed, and *CONC* the corrected concentrations of the analyzed elements, followed by those assumed (in this example, oxygen only).

Example: It might be desirable to reset the total to 100 percent. This could be done as

```
      ∇ AJST
[1]     CONC←CONCx100 ÷ +/CONC   .
      ∇
```

Example: A more complex problem would be resetting the oxygen content of an amphibole on the basis of corrected major element concentrations, apparent F concentration, assumed (OH) content, and a Fe^{2+}/Fe^{3+} ratio that has been determined previously by wet chemistry. It could be accomplished as

```
    ∇ AJST
[1]  CONC[11]←((+/FACxCONC)-+/CONC[⍳10])
         -((0.42107xCONC[13])+0.22564xCONC[9])
         +((1.2865xCONC[5])-FE2)x0.11134 ,
    ∇
```

where *FAC←1.3992, 1.6680, 1.3478, 1.8895, 1.2865, 1.6581, 2.1393, 1.2046, 1, 1.2912, 0, 8.9364, 1* and the order of data input for the analyzed elements and the assumed elements was Ca, Ti. Na, Al, Fe, Mg, Si, K, Cl, Mn, O, H, F. *FE2* is the weight percent of FeO.

Table 4.- Analysis lines and code numbers.

Element	Atomic No. Specifies Vector "ZL"	Atomic Weight Specifies Vector "A"	Wavelengths (in Å)		Critical Excitation Voltage Specifies CEXVO	Line Code No.
			$\lambda K\alpha$	$\lambda L\alpha_1$		
Na	11	22.9898	11.89		1.1	1
Mg	12	24.312	9.87		1.3	2
Al	13	26.9815	8.32		1.6	3
Si	14	28.086	7.11		1.8	4
P	15	30.9738	6.14		2.1	5
S	16	32.064	5.36		2.5	6
Cl	17	35.453	4.72		2.8	7
Ar	18	39.948	4.193		3.2	-
K	19	39.102	3.73		3.6	8
Ca	20	40.08	3.35		4.0	9
Sc	21	44.956	3.02		4.5	10
Ti	22	47.90	2.74		4.964	11
V	23	50.942	2.50		5.5	12
Cr	24	51.996	2.29		5.989	13
Mn	25	54.938	2.10		6.537	14
Fe	26	55.847	1.93		7.111	15
Co	27	58.933	1.79		7.709	16
Ni	28	58.71	1.65		8.331	17
Cu	29	63.54	1.54		8.981	18
Zn	30	65.37	1.43		9.961	19
Ga	31	69.72	1.34		10.4	20
Ga	31	69.72		11.318	1.3	36
Ge	32	72.59	1.25		11.1	21
Ge	32	72.59		10.456	1.4	37
As	33	74.922	1.17		11.8	22
As	33	74.922		9.671	1.5	38
Se	34	78.96	1.10		12.7	23
Se	34	78.96		8.99	1.7	39
Br	35	79.909	1.04		13.4	24
Br	35	79.909		8.375	1.8	40
Rb	37	85.47	.92		15.2	25
Rb	37	85.47		7.318	2.1	41
Sr	38	87.62	.87		16.1	26
Sr	38	87.62		6.862	2.2	42
Y	39	88.905	.83		17.1	27
Y	39	88.905		6.448	2.4	43
Zr	40	91.22	.78		18.0	28
Zr	40	91.22		6.057	2.5	44
Nb	41	92.906	.75		19.0	29
Nb	41	92.906		5.712	2.7	45
Mo	42	95.94	.71		20.0	30
Mo	42	95.94		5.395	2.9	46
Tc	43	99	.67		21.1	31
Ru	44	101.07	.64		22.1	32
Ru	44	101.07		4.836	3.2	47
Rh	45	102.905	.61		23.2	33
Rh	45	102.905		4.588	3.4	48
Pd	46	106.4	.58		24.4	34
Pd	46	106.4		4.359	3.6	49
Ag	47	107.870	.56		25.5	35
Ag	47	107.870		4.146	3.8	50
Cd	48	112.40		3.948	4.0	51
In	49	114.82		3.764	4.2	52
Sn	50	118.69		3.592	4.4	53
Sb	51	121.75		3.423	4.7	54
Te	52	127.60		3.282	5.0	55
I	53	126.904		3.142	5.2	56
Xe	54	131.30		3.016	5.5	-
Cs	55	132.905		2.886	5.7	57
Ba	56	137.34		2.770	6.0	58
La	57	138.91		2.660	6.3	59
Ce	58	140.12		2.556	6.6	60
Pr	59	140.907		2.458	6.8	61
Nd	60	144.24		2.365	7.1	62
Pm	61	147		2.278	7.4	63
Sm	62	150.35		2.195	7.7	64
Eu	63	151.96		2.116	8.1	65
Gd	64	157.25		2.042	8.4	66
Tb	65	158.924		1.972	8.7	67
Dy	66	162.50		1.905	9.1	68
Ho	67	164.430		1.841	9.4	69
Er	68	167.26		1.680	9.8	70
Tm	69	168.934		1.723	10.1	71
Yb	70	173.04		1.668	10.5	72
Lu	71	174.97		1.616	10.9	73
Hf	72	178.49		1.566	11.3	74
Ta	73	180.948		1.519	11.7	75
W	74	183.85		1.473	12.1	76
Re	75	186.2		1.433	12.5	77
Os	76	190.2		1.389	13.0	78
Ir	77	192.2		1.349	13.4	79
Pt	78	195.02		1.310	13.9	80
Au	79	196.967		1.274	14.4	81
Hg	80	200.59		1.239	14.8	82
Tl	81	204.37		1.205	15.3	83
Pb	82	207.19		1.173	15.9	84
Bi	83	208.980		1.142	16.4	85
Po	84	210		1.114	16.9	86
At	85	210		1.085	17.5	-
Rn	86	222		1.057	-	-
Fr	87	223		1.03	18.7	87
Ra	88	226		1.0046	19.2	-
Ac	89	227		.9779	19.8	-
Th	90	232.038		.954	20.5	88
Pa	91	231		.9328	21.1	89
U	92	238.03		.9105	21.8	90

CALC (called by *CC*←*0*)

This dummy subroutine is provided so that calculations such as those for structural formulae of minerals, adjustments of composition to 100 percent (perhaps on a water-free basis), determination of the CIPW norm, printout of the weight percentages of the constituent oxides, and so on, may be made after all corrections have been performed.

Example: It might be desirable to have the composition of a glass recalculated to 100 percent in terms of the oxides, on a water-free basis. A suitable program would be

```
     ∇ CALC
[1]    CONC←CONCxOXFACx100÷+/CONCxOXFAC
[2]    'THE WEIGHT PERCENTS OF THE OXIDES ARE:'
[3]    CONC,+/CONC
     ∇
```

where *OXFAC* had been defined previously outside the program as a vector containing the oxide conversion factors for each of the elements analyzed (+ those assumed), with zeros inserted to set assumed oxygen and hydrogen concentrations to zero. Thus if the elements present and their concentrations were

Si	Ti	Al	Fe	Mg	Ca	Na	K	O	H
33.0	0.3	7.7	1.5	0.3	1.1	3.6	2.2	49.8	.03

OXFAC would be

2.1393, 1.6680, 1.8895, 1.2865, 1.6581, 1.3992, 1.3478, 1.2046, 0, 0

and the corrected output (rounded to 2 decimal places) would be

72.69, 0.52, 14.98, 1.99, 0.51, 1.58, 5.00, 2.73, 0, 0, 100

CONVERGENCE OF CORRECTIONS

The degree of convergence demanded of the newly corrected concentrations and the previously corrected concentrations is controlled by statement [*37*] of *PROBEDATA* . In the program as it is reproduced here (see the Appendix), it is stipulated that if the newly corrected values differ by more than 0.01 percent, the corrections must be recomputed. This condition may be modified, however, by the user simply replacing the 0.01 in statement [*37*] by some other value. Alternatively the 0.01 could be replaced by some expression such as 0.01 x *CONC[EC]*- which would specify that the values must not differ by more than 0.01 (or some other) percentage of the amount present. Similarly other criteria could be chosen and entered by the appropriate modification of statement [*37*].

An automatic exit is built into statement [*39*]. Thus if for some reason corrected concentrations fail to converge (usually due to an error on the part of the user in the input of data) the program will terminate after 100 passes through atomic number, absorption and fluorescence correction loops. The number 100 is completely arbitrary and could be changed by the user. The actual number of passes through this loop for a particular analysis will depend on the number of elements analyzed, the size of the corrections and the convergence demanded of the corrected values. However, 100 is well in excess of the number of loops to be expected for even complex specimens containing a dozen or more elements for which it is stipulated that the corrected values must converge within 0.01 percent.

DEAD-TIME CORRECTIONS

The dead-time correction has been included as an optional facility because with modern instruments it is negligible if the counting rates are low or the counts for the specimen and standard(s) are similar. To activate the dead-time facility, one or more of the elements of the vector *DTC* (see input format sheet, Fig. 2) must be specified as other than zero. The input format sheet allows for *DTC* values for four channels, but more or less can be used depending upon the number of channels used in the analysis and upon the particular instrumental facilities. The actual values for each of the channels must be found experimentally. The formula that has been used to compute the dead-time correction in this program is

$$C_t = C_o/(1 - C_o \times DTC) \ ,$$

where

C_t is the true counting rate

C_o is the observed counting rate, and

DTC is the dead-time constant required and is actually the time interval after a pulse during which the counter cannot respond to a later pulse (also see note under *DTC* in the Appendix).

This probably corrects for the dead-time of the counter reasonably accurately. However with most modern counters the dead-time is commonly small at all count rates likely to be encountered in routine analysis. On the other hand the dead-time of the electronic systems probably cannot be neglected if the counting rates for specimen and standard are different and the count rates are high. There is good evidence to suggest that the expression given does not apply strictly to electronic dead-time (see Short, 1966; Beaman, Isasi, and Lewis, 1969). The most satisfactory approach is undoubtedly an empirical one; a user can experimentally determine the dead-time for each of the channels on the instrument, as per the manufacturer's instructions, and fit an expression to the results. To use this empirically determined expression a certain amount of modification will be required to *READATA* (statements *[30]* and *[31]* certainly, and possibly also statement *[28]*). The authors will be glad to advise individuals having difficulty in incorporating their expressions for dead-time into the program.

MULTIPLE ANALYSES

When a series of specimens have been analyzed against the same set of standards (e.g. a group of feldspars, or perhaps a series of points within an individual mineral grain), an optional loop can be activated which allows the input of new data for the specimen (and new intensity data for the standards). This avoids repetitive inputting of information that remains unchanged, and, more important from the point of view of computer-time consumed, it avoids the continual recalculation of correction factors which remain constant for particular standards. This loop is activated by specifying *NOSP* by the number of specimens that are to be corrected. If the variable *NSTD* is specified as zero, the program also will call for new intensity data for the standards. If *NOSP* is to be specified as zero, this must be done before the program is called. On the other hand, *NSTD* may be specified as zero at the time when the program calls for new data; prior specification will result in an error in the corrections computed. When *NOSP* (no. of specimens) and *NSTD* (new standard data) are not specified, they will automatically be set to one, and both of the loops will be inactive. In general, it should be noted that variables (see Fig. 2 and Appendix) that may not be changed for new specimens are: *EL, OPVO, P* and *NES*; *NOL* and *NOB* may be changed only if new intensity data for the standards require it. Concentrations and atomic numbers of elements present in the standards may under no circumstances be altered.

CHANGES FOR USE WITH DIFFERENT INSTRUMENTS

The electron microprobes marketed by the different manufacturers all have different take-off angles for the x-rays. This angle (θ) appears in the expression for the absorption correction in the form of cosec θ. For the ARL EMX microprobe used by the authors, $\theta = 52.5°$ and thus cosec $\theta = 1.2605$. If a different instrument is used, the correct value for cosec θ must be inserted in statements *[19]* and *[20]* of *PROBEDATA* . Cosec θ also is involved in the fluorescence corrections, but its correct specification within *PROBEDATA* insures the correct value being used in the *FLC* subroutine which calculates the fluorescence corrections. In the AEI SEM2 and in early CAMECA instruments the take-off angle changes with the glancing angle in the crystal monochromator. This problem in addition to other changes in the atomic number, fluorescence and absorption correction must be dealt with before the program can be used. It cannot be overcome simply by determining the change of angle with wavelength, because this precludes the use of second order lines. It would probably be best to insert the correct values for cosec θ into a new variable, say *COTHETA* , in the order in which the data are input for the specimen. Statements *[19]* and *[20]* of *PROBEDATA* could be rewritten to include *COTHETA[EL]* in the place of 1.2605.

The analysis lines used by the authors together with their code numbers are listed in Table 4. Users of some instruments may wish to utilize other analysis lines. In this situation a number of changes will be required within the main workspace and also in the ancillary workspaces containing the banks of mass absorption coefficients. The coefficients listed there are those corresponding to the wavelengths of all the analysis lines (see Table 4). Thus in setting up the tables it is necessary to decide what lines are likely to be used for analysis; the matrix then may be filled with the coefficients to be used (those of Heinrich (1966) are recommended). A code number then must be assigned to each of these lines and before *PROBEDATA* can be implemented, the vector *EL* must be specified by a list of code numbers in the same order in which the data for the elements are entered. The code numbers are used within the program to call the correct values for the critical excitation voltages from the vector *CEXVO* . Thus once the analysis lines have been chosen, the appropriate mass absorption coefficients stored and code numbers assigned, *A, CEXVO* and *ZL* must be specified in the order of the code numbers by the atomic weights, critical excitation voltages in KeV and atomic numbers respectively for all lines. The critical excitation voltages that are used are those tabulated by Birks (1963); they are listed in Table 4.

DETAILED INSTRUCTIONS FOR USE OF PROGRAM

It is assumed that the user now has entered the functions *PROBEDATA, READATA, FLC, MUCO,* ***RND*** and *AJST* in his main workspace. In addition the following variables should have been specified and stored in the same workspace: *A, CEXVO, LNCO, XF, ZL, J* and whereas the following variables are specified immediately prior to the calling of *PROBEDATA*. These then will be stored and remain unchanged until respecified at some time: *DTC, EL, AS, B, CS, D, P, ZEA, ZD, OPVO, NOL, NOB, NES, STCONC, SM, AJ, LL1(2,3,4---), M1(2,3,4---), N1(2,3,4---)*, and *O1(2,3,4---)* . For the program

PROBEDATA INPUT DATA FORM

Enter zeros if dead time corrections need not be computed.

DTC←	CHANNEL 1 $1 x 10^{-6}$	CHANNEL 2 $1 x 10^{-7}$	CHANNEL 3 0	CHANNEL 4 0	(dead time constants given by $C_t=C_o/(1-C_o xDTC)$.

EL← Code nos. of analysis lines of elements determined

1, 15, 25, 44, 76

AS←	No. of peak readings for specimens (must be same for all elements). 2	*B*←	No. of background readings for specimen (must be same for all elements). 2

CS← Peak readings for all elements in same order as *EL* (all readings for 1st element, then 2nd, 3rd, etc.).

100	100	10	10	101	101	11	11	102	102

D← Background readings for all elements in same order as peak readings. (*CS*)

10	10	1	1	11	11	2	2	12	12

P←	No. of standard to which each analysis line is to be referred (1st, 2nd, 3rd, etc.) in same order as *EL*. 1, 2, 1, 2, 1
XEA←	Concentrations of elements present in specimen but not determined. 15
ZD←	Atomic Nos. of assumed elements in same order as for *XEA*. 8
OPVO←	Operating voltage (in KV) at which each element was determined (same order as *EL*). 5, 10, 16, 20, 26.5
NOL←	No. of peak readings for each standard (N.B. for any particular standard the number of peak readings must be the same for all elements analysed). 2, 1
NOB←	No. of background readings for each standard (N.B. for any particular standard the number of background readings must be the same for all elements analysed). 1, 2
NES←	No. of elements determined on each standard (same order *NOL*). 3,2
STCONC←	Concentrations in standards of elements determined (same order as *EL*). 25, 5, 25, 5, 25
SM←	Number of channel used for each element in same order as *EL* (N.B. use only if dead time corrections are to be computed otherwise leave blank). 1, 2, 3, 1, 2
AJ←	Enter 0 if concentrations of assumed elements are to be adjusted via a sub-routine during computation; otherwise leave blank.
CC←	**Enter 0 if corrected concentrations are to be adjusted via a sub-routine (*CALC*) after computation; otherwise leave blank.**

Figure 2.- *PROBEDATA* input data form.

CONCENTRATIONS OF ALL ELEMENTS PRESENT IN STANDARDS

*LL*1←	STD1	25	5	25	5	25	15				
*LL*2←	STD2	25	5	25	5	25	15				
*LL*3←	STD3										
*LL*4←	STD4										
*LL*5←	STD5										
*LL*6←	STD6										

ATOMIC NOS. OF ALL ELEMENTS PRESENT IN STANDARDS
(SAME ORDER AS CONCENTRATIONS LISTED ABOVE)

*M*1←	STD1	11	26	37	40	74	8				
*M*2←	STD2	11	26	37	40	74	8				
*M*3←	STD3										
*M*4←	STD4										
*M*5←	STD5										
*M*6←	STD6										

PEAK READINGS FOR ELEMENTS DETERMINED IN STANDARDS
(FOR A PARTICULAR STANDARD ORDER IS AS IN *P* - SEE PREVIOUS PAGE)

*N*1←	STD1	100	100	101	101	102	102				
*N*2←	STD2	10	11								
*N*3←	STD3										
*N*4←	STD4										
*N*5←	STD5										
*N*6←	STD6										

BACKGROUND READINGS FOR ELEMENTS DETERMINED IN STANDARDS
(ORDER AS IN PEAK READINGS ABOVE)

*O*1←	STD1	10	11	12							
*O*2←	STD2	1	1	2	2						
*O*3←	STD3										
*O*4←	STD4										
*O*5←	STD5										
*O*6←	STD6										

ADDITIONAL INFORMATION.: e.g. *AJST* and/or *CALC* SUBROUTINES; *X*←, etc.

MABSCO SHOULD BE:

4109.1	24.5	3.1	1040.8	614.3	11.4
500.0	57.2	7.3	2335.1	1385.9	26.8
10166.8	71.4	78.0	2690.5	1614.9	276.2
3824.8	206.1	27.6	1078.3	3958.2	98.1
4878.2	257.2	34.4	1375.3	845.8	122.4
4794.0	305.7	189.5	1626.3	3674.6	150.8

YA 11, 26, 37, 37, 40, 74

YB 37, 40, 74

5 loops

as it is reproduced here (see the Appendix), mass absorption coefficients for all the various analysis line wavelengths have been stored in ancillary workspaces (WS) as

WS-1...coefficients for all wavelengths corresponding to code nos. 1-35.

WS-2...coefficients for all wavelengths corresponding to code nos. 36-64.

WS-3...coefficients for all wavelengths corresponding to code nos. 65-90.

In addition, WS-1 should contain `APLOADA`, WS-2 `APLOADB`, and WS-3 `APLOADC`. At this point the following operations should be carried out to run the program (see the Appendix for dummy test data):

1. Command: `) LOAD WS-1`

2. Command: `X←`vector of atomic numbers of all elements listed as present in the specimen and all standards- in any order (also, duplication does not matter)

3. Command: `APLOADA`

   Response: `LOADA READY` -possibly followed by: `NO MORE MABSCO VALUES REQUIRED`

4. Command: `) SAVE WS-1`

   At this point if the response to 3. above was `NO MORE MABSCO VALUES REQUIRED`, omit steps (5)-(12) and continue at (13). Otherwise proceed to 5.

5. Command: `) LOAD WS-2`

6. Command: `) COPY WS-1 LOADA`

7. Command: `APLOADB`

   Response: `LOADA READY` -possibly followed by: `NO MORE MABSCO VALUES REQUIRED`

8. Command: `) SAVE WS-2`

   At this point if the response to 7. was `NO MORE MABSCO VALUES REQUIRED`, omit steps (9)-(12) and continue at (13). Otherwise proceed to 9.

9. Command: `) LOAD WS-3`

10. Command: `) COPY WS-2 LOADA`

11. Command: `APLOADC`

    Response: `LOADA READY`

12. Command: `) SAVE WS-3`

13. Command: `) LOAD WS-4` -main workspace containing `PROBEDATA` , etc.

14. Command: `) COPY WS-3 LOADA`

15. Command: `MUCO`

    Response: **`MABSCO READY`**
    At this point specify all the variables listed in `PROBEDATA` input sheet by the applicable scalar or vector quantities

16. Command: `PROBEDATA`

    Response: `TYPE VALUES OF 1 [1]`
    □:enter `LL1`

    Response: `TYPE VALUES OF 2 [1]`
    □:enter `M1`

    Response: `TYPE VALUES OF 3 [1]`
    □:enter `N1`

    Response: `TYPE VALUES OF 4 [1]`
    □:enter `O1`

    At this point the program will either call for the data for the second standard (`TYPE VALUES OF 1 [2]`, etc., etc.) and then the third and so on or, if all the data for the standards have been input, it will carry on. If deadtime corrections are not required the next step will automatically be omitted otherwise. . . . .

    Response: `TYPE 5:`
    □:enter vector specifying `SM`

    Response: Corrected counts for standard will be printed out

    Response: Corrected counts for specimen will be printed out

    Response: `APPARENT CONCENTRATIONS ARE:` - followed by a list of the concentrations corrected for background (and deadtime if this has been requested) in the order of the input data, followed by the concentrations of assumed elements and then the total. At this point the program enters the main part of *PROBEDATA* and will print out only the value of a loop counter as the successive iterations of the atomic number, absorption and fluorescence corrections are performed. When satisfactory convergence has been obtained for all elements the program will carry on to print out:

Response: *CORRECTED CONCENTRATIONS ARE [ORDER:*(list of elements)*]:-* followed by a list of element concentrations (in the same order as the apparent concentrations) corrected for atomic number, absorption and fluorescence effects, followed by the concentrations of assumed elements (modified by *AJST* if it was called) and then the total. If the subroutine *AJST* has been defined and called, any adjustments specified therein will also have been made.

Response: *Z-CORRECTIONS ARE:* -followed by a list of atomic number corrections in the same order as the concentrations of the elements. These are the factors by which the apparent concentrations must be multiplied to take account of atomic number effects in both specimen and standard.

Response: *ABSORPTION CORRECTIONS ARE:* followed by a list of absorption corrections in the same order as the concentrations of the elements. These are the factors by which the apparent concentrations must be multiplied to take account of absorption effects in both specimen and standard.

Response: *FLUORESCENCE CORRECTIONS ARE:* - followed by a list of fluorescence corrections in the same order as the concentrations of the elements. These are the factors by which the apparent concentrations must be multiplied to take account of fluorescence effects in both the specimen and standard.

At this point the program will either:

1. Terminate its operation or
2. If the subroutine *CALC* has been defined and called it will carry out further manipulation of the corrected data; it might be instructed to calculate a structural formula for the mineral, or print out concentrations in the form of weight percentages of the constituent oxides, or calculate the CIPW norm, etc.

If the variable *NOSP* has been specified as other than 1, the program will call for new data for the next specimen. If *NSTD* is specified at this time as zero, new standard data will be called. If data for another specimen is to be input or intensity data for the standard is to be changed following any printout that there may have been from the *CALC* subroutine, the following procedure will apply:

Response: *TYPE DATA FOR NEXT SPECIMEN:*
⎕:
At this point enter data in the following form:
for example
CS←
(new values). . . . . .

Response: ⎕:
XEA← (new values)

Response: ⎕:
D← (new values)

3 opportunities are provided for input of new specimen data. If it is found commonly that this is insufficient,

another ⎕ may be added to statement *[51]*. If no further data need be added after the first ⎕ has appeared, the remaining ⎕'s may be satisfied by simply respecifying any variable as itself (e.g. *B←B*). If new standard data also are to be input, the computer then will respond by initiating the loop that follows command 16 above; this will be terminated when all the new intensity data for the standards have been specified (and the data on concentrations respecified by themselves). The program now will carry on from the termination of this loop to calculate the new concentrations and new corrections - and then, if required, will call for the next batch of specimen (and/or standard) data.

(N.B. If the program is terminated prematurely at any time, it is essential to make certain that the variable *BP←0* before proceeding to rerun it .)

EDITING AND MODIFICATIONS

The main program and most subroutines have been written with labelled statements so that extra statements may be inserted at almost any point without the danger of interfering with addresses. This procedure is less economical of space but allows the user to make modifications.

Operation of the program may be interrupted at any time simply by hitting the "ATTN" key on the terminal, this resulting in the statement number and the function name at the time of interrupt being printed out. The value of variables then may be displayed to investigate the cause of long delays in the output of corrected concentrations. The operation of the program can be continued after such an interrupt by typing *→N* where *N* is the number of the statement at which the operation was interrupted.

A printout of each new value of the loop counter has been included. The main purpose of this is to indicate to the user that the program is operating normally (a new value should be printed every few seconds). If this printout is not requested (the ⎕← could be deleted from statement *[11]*) it can be difficult to distinguish between a long correction process involving many iterations, and a computer failure.

Errors may be made in the inputting of data for the standards to the loop in *READATA* (an incorrect value may be accidentally typed). If this happens, the operation of the program may be terminated at this point by answering the next ⎕ (input request) with "→". The program then may be called again for the input of correct information. The values of variables such as *AJ, ZD, NOSP* (which are reset at the end of the program) will not be affected by this premature termination and thus need not be respecified before calling *PROBEDATA* again.

ADVANTAGES AND DISADVANTAGES OF AN APL LANGUAGE PROGRAM

The principal advantage of this APL language program is that it can be used from a remote terminal conveniently situated with respect to the electron probe to give corrected values for the composition of the material quickly. The minimum amount of data need be input, and in particular, all mass absorption coefficients required are selected and assembled simply by specifying the atomic numbers involved. This applies to all elements and not only a dozen or so more common elements, as is the situation with some FORTRAN programs available. No key punching operations are necessary and errors in the physical process of inputting information via the typewriter terminal become apparent almost immediately when the appropriate error message is sent by the computer. The experimental conditions under which the electron probe has been operating can be maintained essentially constant until the corrected output has been checked. The language itself is concise (about 200 statements for the main program and all subroutines). Optional subroutines may be written, if necessary on the spot, for further manipulation of the corrected output data; these are easily incorporated into the body of the program in one or other of the 'slots' provided. Furthermore, the program may be used by a person with only cursory knowledge of the language and its operation, by following the step-by-step directions. The whole program including all the subroutines, functions, matrices and constants, as well as the mass absorption coefficients actively in use by the program, can be stored within one workspace of 32K bytes. Only the large banks of mass absorption coefficients from which those needed in a particular analysis are drawn, need ancillary storage (3 workspaces). Thus this program is particularly well suited for use in a laboratory where an electron probe is making analyses of a wide range of different materials requiring many changes in the mass absorption coefficients to be used for correction procedures, and probably different manipulation of the corrected output. APL has the added advantage of ease of editing, so that changes in the main program or any of the subroutines, for the purpose of incorporating extra facilities, modifying correction formulae or entering the latest data for constants etc., are easily and quickly made.

The main disadvantages lie in the fact that APL is an interpretive language and thus is expensive of CPU time. The program outlined above could, in a complex situation involving several standards and a specimen all of which contained many elements, take a minute or more of CPU time to run; a FORTRAN IV program would accomplish the corrections in a matter of seconds. This is unlikely to be of importance to the analyst in terms of time delay, and is undoubtedly compensated for in most situations by the time saved in data input and ancillary manipulation of corrected data. However where CPU time is chargeable and the capacities of an existing computer facility operating in the time-sharing mode are already heavily utilized, the extra time required for interpretive execution may be of considerable significance.

This program does not provide for the input of data in a wide range of formats. It is possible to enter all the readings for peaks and backgrounds output by the electron probe for both specimen and standard (and have the computer do the averaging), but there is the restriction that there must be the same number of peak and of background readings for all elements analyzed. The number of peak readings and the number of background readings, however, may differ from one another. The same restriction applies to any one particular standard. This restriction has not been eliminated for reasons of conciseness and space and also because it is believed that little is to be gained by typing a large number of data into the program simply for averaging purposes.

Where large batches of data from a series of specimens are produced routinely, using the same standards, it will probably be more satisfactory to use a program such as EMPADR V, which was developed by Rucklidge (1967) and Rucklidge and Gasparrini (1968). The correction factors for the standards may be computed once and then stored for repeated use. In some laboratories the correction factors, once computed, are stored on cards, to be inserted into the programs whenever the particular standards are again utilized. Space limitations do not permit this type of permanent storage for an APL program. However, during one particular run, the correction factors for the standards in use at that time are computed only once and then stored temporarily until the operation of *PROBEDATA* finally terminates.

REFERENCES

Beaman, D.R., Isasi, J.A., and Lewis, R., 1969, The source and nature of dead-time in electron microprobe analysis: Proc. 4th Nat. Conf. Electron Microprobe Analysis, Pasadena, Paper 13, 4 p.

Birks, L.S., 1963, Electron probe microanalysis: John Wiley & Sons, Inc., New York, 253 p.

Duncumb, P., and Reed, S.J.B., 1968, The calculation of stopping powder and backscatter effects in electron probe microanalysis, in Quantitative electron probe microanalysis: Nat. Bur. Standards, Sp. Publ. 198, p. 133-154.

Duncumb, P., and Shields, P.K., 1966, Effect of critical excitation potential on the absorption correction, in The electron microprobe: John Wiley & Sons, Inc., New York, p. 284-295.

Duncumb, P., Shields-Mason, P.K., and Da Casa, C., 1968, Accuracy of atomic number and absorption corrections in electron probe microanalysis: 5th Intern. Cong. X-ray optics & microanalysis, Tubingen (proceedings to be published by Springer).

Falkoff, A.D., and Iverson, K.E., 1968, APL\360 user's manual: IBM, White Plains, New York, 132 p.

Heinrich, K.F.J., 1966, X-ray absorption uncertainty, in The electron microprobe: John Wiley & Sons, Inc., New York, p. 296-377.

Heinrich, K.F.J., 1967, The absorption correction model for microprobe analysis: Trans. 2nd Nat. Conf. Electron Microprobe Analysis, Boston, Paper 7, 2 p.

Keil, K., 1967, The electron microprobe x-ray analyzer and its application in mineralogy: Fortschr. Miner, Bd. 44, Heft 1, p. 4-66.

Long, J.V.P., 1967, Electron probe microanalysis, in Physical methods in determinative mineralogy: Academic Press, London, p. 215-260.

Philibert, J., 1963, A method for calculating the absorption correction in electron probe microanalysis, in X-ray optiocs and x-ray microanalysis: Academic Press, New York, p. 379-392.

Reed, S.J.B., 1965, Characteristic fluorescence corrections in electron-probe microanalysis: British Jour. Appl. Phys., v. 16, p. 913-926.

Rucklidge, J.C., 1967, A computer program for processing microprobe data: Jour. Geology, v. 75, no. 1, p. 126.

Rucklidge, J.C., and Gasparrini, E.L., 1968, EMPADR V: specifications of a computer program for processing electron microprobe analytical data: Dept. Geology, Univ. Toronto Publ., 31 p.

Short, M.A., 1966, Detection and correction of non-linearity in x-ray counting systems: 5th Conf. on x-ray analytical methods, Swansea, p. 60-62.

Smith, J.V., 1965, X-ray emission microanalysis of rock-forming minerals: I -experimental techniques: Jour. Geology, v. 73, no. 6, p. 830-864.

Sweatman, T.R., and Long, J.V.P., 1969, Quantitative electron-probe microanalysis of rock-forming minerals: Jour. Petrology, v. 10, pt. 2, p. 332-379.

APPENDIX

```
     ∇ PROBEDATA;A̲;ALSP;ALST;B̲;C;C̲;CT;CV;D̲;E̲;F;H;K;KK;KT;OV;P̲;PP;Q̲;RFAC;SIG;T;VV;Z̲
[1]    STMU←ALST←SIG←NFC←STFC←NUMρ+/H←(1+NO←⌈/(P←,P))ρ0×+/OPVO←0 RND,OPVO×NUM÷NUM←ρ(EL←,EL)
[2]    READATA
[3]    SIG←(4.5×10*5)÷(OPVO*1.65)-(CEXVO[EL])*1.65
[4]    EC←PP←K←0
[5]    NUC←CONC←ACONC×NUM÷+/ZCOR←ABC←NUMρ1
[6]    L99:→((BP÷NSTD)=K÷K←K+1+KT←0)/L29
[7]    L8:→(STZM[K;KT←KT+1]=0)/L95
[8]    H[K+1]←+/1.2×(A[A̲]÷(A̲←STZM[K;⍳(KK-1)])*2)×A̲÷+/A̲←STM[K;⍳(KK-1)]×KK÷KK←(STZM[K;],0)⍳0
[9]    L95:→(K<NO)/L99
[10]   L29:EC←0
[11]   L7:H[1]←K←KT←SPMU←EC-EC←EC+PP÷⎕←PP←PP+1
[12]   ALSP←K←CN←0×H[1]←+/1.2×(A[Z]÷Z*2)×CONC÷+/CONC
[13]   L55:→((YA[CN←CN+1]≠Z[EC]),KT=1)/L55,L56
[14]   →((YA[CN]>38),YA[CN]>34×KT←1)/L56,L55
[15]   L56:K←C←CT←0
[16]   L11:→(0≠ALSP←+/((T÷A[T])×●(VV←583×((OV←OPVO[EC])+CV←CEXVO[EL[EC]]))÷J[T←Z])×CONC÷+/CONC)/L22
[17]   L23:ALST[EC]←+/((T÷A[T])×●VV÷J[T←STZM[PE;⍳K]])×STM[PE;⍳K]÷+/STM[PE;]×K÷K←¯1+STZM[PE←P[EC];]⍳0
[18]   L22:→(C=1+0×+/KK←X⍳T)/L25
[19]   →(0≠SPMU←+/MABSCO[KK;CN]×CONC÷+/CONC÷1.2605)/L21
[20]   L25:→(0≠STMU[EC]←+/MABSCO[KK;CN]×STM[PE;⍳K]÷(+/STM[PE;])÷1.2605)/L27
[21]   L21:→((ALST[EC]≠K←¯1+C←1),ALST[EC]=0)/L91,L23
[22]   L27:→(0≠Z̲←+/STZM[PE;]×STM[PE;]÷+/STM[PE;])/L1
[23]   L91:C←Z̲-Z̲←+/(Z×CONC)÷+/CONC×PE÷PE←P[EC]
[24]   L1:→(0≠Q̲×F÷F←1+E̲←Z̲÷10×B̲÷B̲←P̲←1+Q̲←⌊U̲×10×U̲÷U̲←CV÷OV)ρ2+⌶26
[25]   Q̲←0.1
[26]   RFAC←D̲+((A̲+((B̲←R[⌊F;B̲+1])-A̲←R[⌊F;B̲])×(U̲-Q̲)÷P̲-Q̲)-D̲←(C̲+((D̲←R[⌈F;B̲+1])-C̲←R[⌈F;B̲])×(U̲-Q̲)÷(P̲←P̲÷10)-Q̲←Q̲÷10))×(⌈E̲)-E̲
[27]   →(C=1)/L5
[28]   →(0≠ALSP←ALSP÷RFAC)/L19
[29]   L5:ALST[EC]←ALST[EC]÷RFAC
[30]   L92:→(C=1)/L91
[31]   L19:ZCOR[EC]←ALSP÷ALST[EC]
[32]   ABC[EC]←((1+B̲)÷(1+A̲÷D̲)×1+(B̲←H[1+PE])×1+(A̲←STMU[EC])÷D̲)÷(1+C̲)÷(A̲)×1+(C̲←H[1])×A̲←1+SPMU÷D̲←SIG[EC]
[33]   NUC[⍳NUM]←ACONC[⍳NUM]×ABC×ZCOR
[34]   FLC
[35]   →(AJ≠0)/L6
[36]   AJST
[37]   L6:→((|NUC[EC]-CONC[EC])>0.01)/L10
[38]   →((EC<NUM),NUM=EC×CONC[EC]÷CONC[EC]←NUC[EC])/L7,L12
[39]   L10:→(PP<100×CONC[EC]÷CONC[EC]←NUC[EC])/L29
[40]   L12:('CORRECTED CONCENTRATIONS ARE: [ORDER:';(3×ρ(,Z))ρ(ZSYM[Z;]);']')
[41]   ⎕←3 RND CONC,+/CONC
[42]   'Z-CORRECTIONS ARE:'
[43]   ⎕←4 RND ZCOR
[44]   'ABSORPTION CORRECTIONS ARE:'
[45]   ⎕←4 RND ABC
[46]   'FLUORESCENCE CORRECTIONS ARE:'
[47]   →(CC≠0×+/⎕←4 RND CONC[⍳NUM]÷ABC×ZCOR×ACONC[⍳NUM])/L4
[48]   CALC
[49]   L4:→(0=NOSP←NOSP-1)/L9
[50]   'TYPE DATA FOR NEXT SPECIMEN'
[51]   ⎕,⎕,⎕
[52]   →(100≠BP←1×NSTD)/2
[53]   L9:ZD←⍳BP←0×NOSP←NSTD←AJ←CC←1
     ∇
```

```
      ∇ READATA;CT;E;F;G;K;R;S;SM
[1]     E←(NUM,B)ρ(,D)×NO÷NO←⌈/(,P)×NUM÷NUM←ρ(,EL)
[2]     F←(NUM,AS)ρ(,CS)
[3]     G←(2,NUM)ρK←0
[4]     L2:G[2;K]←((+/F[K;])÷AS)-(+/E[K←K+1;])÷B
[5]     →(G[2;K]>0)/L13
[6]     G[2;K]←0
[7]     L13:→((K<NUM),BP=1)/L2,L98
[8]     F←⍳1-E←1
[9]     F←F,(E=P)/⍳ρP
[10]    →(NO≥E←E+1)ρ¯1+⌶26
[11]    NES←,NES×(ρNOL)÷ρNOL←,NOL×(ρNOB)÷ρNOB←,NOB
[12]    STM←STZM←(NO,20)ρK←CT←0
[13]    L52:('TYPE 1 [';K←K+1;']')
[14]    STM[K;]←E,(20-ρE←,⎕)ρ0
[15]    ('TYPE 2 [';K;']')
[16]    STZM[K;]←E,(20-ρE←,⎕)ρ0
[17]    ('TYPE 3 [';K;']')
[18]    S←(NES[K],NOL[K])ρE←,⎕
[19]    ('TYPE 4 [';K;']')
[20]    R←(NES[K],NOB[K])ρE←,⎕
[21]    ACONC←NUMρE←0
[22]    L51:G[1;F[CT←CT+1]]←((+/S[E;])÷NOL[K])-(+/R[E←E+1;])÷NOB[K]
[23]    →(G[1;F[CT]]>0)/L58
[24]    G[1;F[CT]]←G[2;F[CT]]←0
[25]    ('NO COUNTS FOR STD ELEMENT ';F[CT];'.  SP CONC SET TO 0')
[26]    L58:→(((CT=ρF),E<NES[K]),CT≠ρF)/L53,L51,L52
[27]    L98:G[1;]←G̲
[28]    L53:→((+/DTC)=0)/L59
[29]    'TYPE 5'
[30]    SM←DTC[SM←,⎕]
[31]    →(BP≠ρρρG←G÷1-G×SM[(2,NUM)ρ⍳NUM])/L59
[32]    G[1;]←G̲
[33]    L59:ACONC←G[2;]÷(G̲←G[1;])÷STCONC×(+/ρρG)÷+/ρρ⎕←3 RND G←G+1E¯8
[34]    L3:'APPARENT CONCENTRATIONS ARE:'
[35]    ⎕←3 RND ACONC,(+/ACONC←ACONC,XEA)
[36]    Z←ZL[EL],ZD×XTRA÷XTRA←ρZD←,ZD
      ∇
```

```
      ∇ MUCO;MU;A
[1]     X←,X←((4ρ0),(A[1]ρ1),((+/A[2 3 4])ρ0))/A←LOADA
[2]     YA←,YA←(((4+A[1])ρ0),(A[2]ρ1),((+/A[3 4])ρ0))/A
[3]     YB←,YB←(((4++/A[⍳2])ρ0),(A[3]ρ1),(A[4]ρ0))/A
[4]     MABSCO←⍉MU←((ρYA),(ρX))ρA←(((4++/A[⍳3])ρ0),(A[4]ρ1))/A
[5]     →((¯1×YC←+/(ρYA)-ρYB)≠ρ⎕←'MABSCO READY')/100
      ∇
```

```
      ∇ R←N RND X
[1]     R←(10*-N)×⌊0.5+X×10*N
      ∇
```

```
     ∇ FLC;C;CHK;CL;CO;CT;FC;K;KK;KT;MU;QA;QB;SU;T
[1]    QB←NUC×QA÷QA←Z×CHK÷CHK←NUM+XTRA×C←1
[2]    →((CT←0)≠SU←SPMU×T÷T←Z[EC])/LB
[3]    LN:→(STFC[EC]≠CT←0)/LQ
[4]    NFC[EC]←NUC[EC]+0×+/QB←STM[PE;]×QA÷QA←QB+0×SU←STMU[EC]+CHK-CHK←¯1+(((QB←STZM[PE;]),0)+1)⍳2+C←¯1
[5]    LB:→(QA[CT←CT+1]<FL[T-10;3])/LL
[6]    →(QA[CT]<FL[T-10;K←2])/LG
[7]    LC:→(T<29+CL←6)/LAB
[8]    →(¯1≠ZF←QA[CT]-FL[T-10;1])/LBB
[9]    LAB:ZF←QA[CT]-T
[10]   LBB:KK←X⍳T×KT÷KT←YA⍳QA[CT]
[11]   LW:→(¯1≠FC←QB[CT]×FL[T-10;CL]×(10*XF[OPVO[EC]]×ZF)×MABSCO[KK;KT]÷+/QB)/LY
[12]   LD:→(T<35)/LCB
[13]   →(¯1≠ZF←FL[QA[CT]-10;1]-FL[T-10;1])/LDB
[14]   LCB:ZF←FL[QA[CT]-10;1]-T
[15]   LDB:KT←YB⍳QA[CT]
[16]   →(0≠KK←X⍳T×KT÷KT←KT+YC)/LW
[17]   LY:KK←⍳MU←CO←0
[18]   LE:→(CO<CHK×ρρKK←KK,X⍳QA[CO←CO+1])ρ⌶26
[19]   MU←+/MABSCO[KK;KT]×QB[⍳CHK]÷+/QB
[20]   →((K=3),K=5+0×FC←FC÷MU÷((⍟1+SU÷MU)÷SU÷MU)+(⍟1+CO)÷CO←LNCO[OPVO[EC]]÷MU)/LH,LK
[21]   →((K=2),K=4+0×NUC[EC]←NUC[EC]×(1÷1+FC)*C)/LI,LL
[22]   LG:→(1≠K←3)/LC
[23]   LH:NUC[EC]←NUC[EC]×(1÷1+FC×0.1)*C
[24]   LI:→(QA[CT]<FL[T-10;5])/LL
[25]   →(QA[CT]<FL[T-10;K←4])/LJ
[26]   →(1≠CL←7)/LD
[27]   LJ:→(¯1≠CL←2+K←5)/LD
[28]   LK:NUC[EC]←NUC[EC]×(1÷1+FC×0.4)*C
[29]   LL:→((CT<CHK),C=1)/LB,LN
[30]   LP:→(¯1≠STFC[EC]←NUC[EC]÷NFC[EC])/100
[31]   LQ:NUC[EC]←NUC[EC]×STFC[EC]
     ∇
```

```
      ∇ APLOADA;K;CT;KT
[1]     YA←YB←LOADA←⍳K←CT←0×⍴X←X[⍋X←,X]
[2]     L7:→((K←K+1)=(⍴X)+1)/L17
[3]     →(((X[K]<11),CT>0),X[K]>38)/L7,L13,L30
[4]     →(¯1≠(YA←,YA←X[K]-10×CT÷CT←CT+1))/L7
[5]     L13:→(X[K]>38)/L17
[6]     YA←YA,X[K]-10
[7]     →((K<⍴X),CT=0)/L7,L30
[8]     L17:KT←0
[9]     L21:→(KT≠(⍴YA×⍴LOADA÷⍴LOADA←LOADA,MABSCO[X;YA[KT←KT+1]]))/L21
[10]    →((¯1×⍴YA←YA+10)≠⍴⎕←'LOADA READY')/1+⌶26
[11]    →(((⌈/X)≤30),L30≠0)/L33,L34
[12]    L30:→(¯1≠⍴⎕←'NO MABSCO VALUES')/L34
[13]    L33:'NO MORE MABSCO VALUES REQUIRED'
[14]    L34:LOADA←(⍴X),(⍴YA),(⍴YB),(⍴LOADA),X,YA,YB,LOADA
      ∇
```

```
      ∇ APLOADB;CT;K;KT;LOADB
[1]     X←((4⍴0),(KT[1]⍴1),((+/KT[2 3 4])⍴0))/KT←LOADA
[2]     YA←,YA←(((4+KT[1])⍴0),(KT[2]⍴1),((+/KT[3 4])⍴0))/KT
[3]     YB←,YB←(((4++/KT[⍳2])⍴0),(KT[3]⍴1),(KT[4]⍴0))/KT
[4]     LOADA←(((4++/KT[⍳3])⍴K←CT←0),(KT[4]⍴1))/KT
[5]     L2:→((K←K+1)=(⍴X)+1)/L11
[6]     →(((X[K]<31),CT>0),X[K]>62)/L2,L8,L26
[7]     →(¯1≠(YB←,YB←X[K]-30×CT÷CT←CT+1))/L2
[8]     L8:→(X[K]>62)/L12
[9]     YB←YB,X[K]-30
[10]    L11:→((K<⍴X),CT=0)/L2,L26
[11]    L12:LOADB←⍳KT←0
[12]    →(KT≠(⍴YB×⍴LOADB÷⍴LOADB←LOADB,MABSCOE[X;YB[KT←KT+1]]))/⌶26
[13]    →((¯1×⍴(YB←YB+30)+(⍴LOADA←LOADA,LOADB))≠⍴⎕←'LOADA READY')/1+⌶26
[14]    →(((⌈/X)<63),L26≠0)/L29,L37
[15]    L26:→(¯1≠⍴⎕←'NO MABSCO VALUES')/L37
[16]    L29:→((¯1×YA←YA,YB)≠⍴⎕←'NO MORE MABSCO VALUES REQUIRED')/L37
[17]    L37:LOADA←(⍴X),(⍴YA),(⍴YB),(⍴LOADA),X,YA,YB,LOADA
      ∇
```

```
      ∇ APLOADC;K;CT;KT;LOADC
[1]     X←((4⍴0),(KT[1]⍴1),((+/KT[2 3 4])⍴0))/KT←LOADA
[2]     YA←,YA←(((4+KT[1])⍴0),(KT[2]⍴1),((+/KT[3 4])⍴0))/KT
[3]     YB←,YB←(((4++/KT[⍳2])⍴0),(KT[3]⍴1),(KT[4]⍴0))/KT
[4]     LOADA←,LOADA←(((4++/KT[⍳3])⍴K←CT←0),(KT[4]⍴1))/KT
[5]     L22:→((K←K+1)=(⍴X)+1)/L11
[6]     →(((X[K]<63),CT>0),X[K]>92)/L22,L88,L62
[7]     →(¯1≠(YC←,YC←X[K]-62×CT÷CT←CT+1))/L22
[8]     L88:→(X[K]>92)/L21
[9]     YC←YC,X[K]-62
[10]    L11:→((K<⍴X),CT=0)/L22,L62
[11]    L21:LOADC←⍳KT←0
[12]    →(KT≠(⍴YC×⍴LOADC÷⍴LOADC←LOADC,MABSCOEF[X;YC[KT←KT+1]]))/⌶26
[13]    →(((⍴⎕←'LOADA READY')×⍴LOADA←LOADA,LOADC)≠(¯1×⍴YA←YA,YB←YB,YC+62))/L72
[14]    L62:'NO MABSCO VALUES'
[15]    L72:LOADA←(⍴X),(⍴YA),(⍴YB),(⍴LOADA),X,YA,YB,LOADA
      ∇
```

DUMMY TEST DATA SAMPLE OUTPUT FROM PROBEDATA

```
         PROBEDATA
TYPE 1 [1]
[]:
         LL1           (input of element concentrations for 1st standard)
TYPE 2 [1]
[]:
         M1            (input of corresponding atomic numbers for 1st standard)
TYPE 3 [1]
[]:
         N1            (input of peak readings for elements analysed against 1st standard)
TYPE 4 [1]
[]:
         O1            (input of background readings for elements analysed against 1st standard)
TYPE 1 [2]
[]:
         LL2           (input of element concentrations for 2nd standard)
TYPE 2 [2]
[]:
         M2            (input of corresponding atomic numbers for 2nd standard)
TYPE 3 [2]
[]:
         N2            (input of peak readings for elements analysed against 2nd standard)
TYPE 4 [2]
[]:
         O2            (input of background readings for elements analysed against 2nd standard)
TYPE 5
[]:
       1,2,3,1,2       (input of channel numbers for each of elements analysed - for computation of dead-time)

    90.008        9          90          9          90.001  (counts for standard corrected for background and
    90.008        9          90          9          90.001  (counts for specimen corrected        dead time)
APPARENT CONCENTRATIONS ARE:                                   for background and dead-time)
25  5  25  5  25  15  100 (apparent concentrations in same order as corrected concentrations
1                                                                 below)
2
3                         (no. of element correction cycles performed)
4
5
CORRECTED CONCENTRATIONS ARE: [ORDER: NA FE RB ZR  W  O] (element symbols in order of corrected concentrations)
25  5  25  5  25  15  100     ( corrected concentrations followed by total)
Z-CORRECTIONS ARE:
1  1  1  1  1                 (atomic no. corrections in same order)
ABSORPTION CORRECTIONS ARE:
1  1  1  1  1                 (absorption corrections in same order)
FLUORESCENCE CORRECTIONS ARE:
1  1  1  1  1                 (fluorescence corrections in same order)
    MABSCO                    (N.B. MABSCO. YA, YB & X will not be output unless specifically requested after termination of
                               PROBEDATA; values are listed here for checking purposes only).
  4109.1         24.5            3.1         1040.8         614.3          11.4  table of mass absorption
   500           57.2            7.3         2335.1        1385.9          26.8  coefficients: Columns correspond
 10166.6         71.4           78           2690.5        1614.9         276.2  to elements analysed (order as in
  3824.8        206.1           27.6         1078.3        3958.2          98.1  YA)Rows correspond to elements
  4878.2        257.2           34.4         1375.3         845.8         122.4  present in specimen and all
  4794          305.7          189.5         1626.3        3674.6         150.8  standards (order of increasing
    YA                                                                           atomic no.).
11  26  37  37  40  74        (atomic nos. of elements for which mass absorption coefficients are
    YB                         listed, N.B. if both K&L lines are involved, the line will be listed twice in YA)
37  40  74
    X                         (atomic nos. of elements for which mass absorption coefficients of L
8  11  26  37  40  74          lines are listed)
                              (atomic nos. of all elements present in specimen and all standards)
```

DUMMY MICROPROBE OUTPUT DATA

FIRST RUN	CHANNEL 1	CHANNEL 2	CHANNEL 3
AT.NO.OF ELEMENT	11	26	37
CODE NO.OF LINE	1	15	25
COUNTING TIME			
SAMPLE PEAK			
1-001.000	0000100	0000010	0000101
2-001.000	0000100	0000010	0000101
SAMPLE BACKGROUND			
1-001.000	0000010	0000001	0000011
2-001.000	0000010	0000001	0000011
STANDARD 1 PEAK			
1-001.000	0000100	NOT USED	0000101
2-001.000	0000100	NOT USED	0000101
STANDARD 2 PEAK			
1-001.000	NOT USED	0000010	NOT USED
STANDARD 1 BACKGROUND			
1-001.000	0000010	NOT USED	0000011
STANDARD 2 BACKGROUND			
1-001.000	NOT USED	0000001	NOT USED
2-001.000	NOT USED	0000001	NOT USED

SECOND RUN	CHANNEL 1	CHANNEL 2	CHANNEL 3
AT.NO.OF ELEMENT	40	74	NOT USED
CODE NO.OF LINE	44	76	NOT USED
COUNTING TIME			
SAMPLE PEAK			
1-001.000	0000011	0000102	
2-001.000	0000011	0000102	
SAMPLE BACKGROUND			
1-001.000	0000002	0000012	
2-001.000	0000002	0000012	
STANDARD 1 PEAK			
1-001.000	NOT USED	0000102	
2-001.000	NOT USED	0000102	
STANDARD 2 PEAK			
1-001.000	0000011	NOT USED	
STANDARD 1 BACKGROUND			
1-001.000	NOT USED	0000012	
STANDARD 2 BACKGROUND			
1-001.000	0000002	NOT USED	
2-001.000	0000002	NOT USED	

EXPLANATION OF SOME IMPORTANT VARIABLES

A.......A list of atomic weights of the elements arranged in order of increasing atomic number from Hydrogen to Uranium (Table 4).

ABC.....The absorption correction for the specimen divided by the absorption correction for the standard (using the formula of Philibert (1963).

ACONC...The apparent concentrations of the elements - i.e. the measured concentrations corrected only for background (and dead-time if requested).

ALSP....Initially the stopping power for the specimen which eventually, when it is divided by the appropriate value of *RFAC*, becomes the atomic number factor for the specimen.

ALST....Initially the stopping power for the standard which eventually, when it is divided by the appropriate value of *RFAC*, becomes the atomic number factor for the standard.

AS......The number of line (i.e. peak) readings to be input for each element for the specimen.

B.......The number of background readings to be input for each element for the specimen.

CEXVO...A list of critical excitation voltages for the lines used in analysis, arranged in the order of the code numbers for the analysis lines (Table 4).

CONC....The previous corrected concentrations of the elements analyzed followed by the assumed concentrations. Eventually becomes the final corrected concentrations.

CS......A list of the line readings for the elements analyzed. These are arranged so that all the readings for the first element are followed by all the readings for the second element and these by all the readings for the third element, and so on.

D.......A list of the background readings for the elements analyzed. These are arranged in the same manner as the values for *CS* above.

DTC.....The dead-time constants for the channels. N.B.: if these are based on 1 sec counting rates, all other readings entered (*CS*, *D*, *N*1, *O*1, etc.) must also be based on 1 sec. counting rates.

EC......A counter indicating the number of the element in the order of data input for which corrections are being carried out.

EL......A list of the code numbers of the lines used in the analysis in the same order as the specimen data input.

FC.....The γ term in Reed's (1965) fluorescence correction formula.

FL......A table of fluorescence correction data given by Reed (1965) and reproduced here as Table 1.

G.......A two row matrix containing the specimen and standard counts for all the elements analyzed - corrected for background (and dead-time if requested).

H.......The "h" term of the absorption correction of Philibert (1963) = $\overline{1.2(A/Z^2)}$.

J.......The mean ionization potential term of the Duncumb and Reed (1968) atomic number correction, tabulated by atomic number and reproduced here in Table 2.

*LL*1(2,3,4...)...Concentrations of elements present in standards 1,2,3,4.....

LNCO....A list of Lenard coefficients for various operating voltages, based on the values tabulated by Philibert (1963), and extrapolated back to 1KV (Table 2).

LOADA...A vector containing all the mass absorption coefficients combined from the storage workspaces WS-1, WS-2, WS-3. It also contains information on which coefficients were loaded from each storage WS and on the atomic numbers involved.

MABSCO..Mass absorption coefficients of all elements present in specimen and all standards for wavelengths of all analysis lines - arranged in order of the atomic numbers listed in the variables *YA* & *YB*. This applies to the main workspace that contains *PROBEDATA* etc. However, in WS-1 *MABSCO* is a table of mass absorption coefficients of all elements from Hydrogen to Uranium for wavelengths corresponding to code numbers 1-35 inclusive.

MABSCOE.Mass absorption coefficients of all elements from Hydrogen to Uranium for all wavelengths corresponding to code numbers 36-64 inclusive, stored in matrix form in WS-2.

MABSCOEF...Mass absorption coefficients of all elements from Hydrogen to Uranium for all wavelengths corresponding to code numbers 65-90 inclusive, stored in matrix form in WS-3.

*M*1(2,3,4...)...Atomic numbers of all elements present in standards 1,2,3,4... in the same order as *LL*1 etc.

MU......The average mass absorption coefficients of the specimen or standard for the wavelength of a line producing fluorescence.

*N*1(2,3,4...)...The line readings for each element determined on standards 1,2,3,4..., arranged in the order that they appear in variable *P*.

NES.....A list of the number of elements determined on each standard, arranged in the same order as the standards are numbered (i.e. 1,2,3,4 etc.).

NFC.....The concentrations of the elements analyzed on entering the *FLC* subroutine, and before the fluorescence corrections are applied.

NO......The number of standards used in the analysis.

NOB.....The number of background readings for each standard in the same order as *NES*. (N.B. for any particular standard the number of background readings must be the same for all elements analyzed).

NOL.....The number of line readings for each standard in the same order as *NES*. (N.B. for any particular standard the number of readings must be the same for all elements analyzed).

NOSP....A variable set to indicate how many specimens are being analyzed against this particular set of standards. It is automatically set to 1 unless otherwise specified.

NSTD....A variable which is specified as 0 after calling *PROBEDATA* if new intensity data for the standards are to be input after the first specimen has been corrected.

NUC.....The new, corrected concentrations of the elements analyzed followed by concentrations of assumed elements.

*O*1(2,3,4...)...The background readings for each element determined on standards 1,2,3,4, arranged in the same order as *N*1,*N*2,*N*3,*N*4, etc.

OPVO....The operating potentials of the probe for each element analyzed (in KV) entered in the same order as the intensity data for the specimen.

P.......The number of standard to which each analysis line is to be referred, arranged in the same order as the input of specimen data.

R.......A matrix containing the backscatter coefficients required for the atomic number correction of Duncumb and Reed (1968), arranged with rows corresponding to the atomic number and columns corresponding to overvoltage. Reproduced here as Table 3.

RFAC....The value of *R* for the specimen (and then the standard) obtained by extrapolating from the values given in Table 3 and assuming linear variation between these values.

SIG.....The Heinrich (1967) modification of the Lenard coefficient for the elements analyzed (this is the same for specimen and standard).

SM......A list of the channels used in the determination of each element (in the same order as the data are input for the specimen) which need only be specified if dead-time corrections have to be computed.

SPMU....χ for the specimen - i.e. the mass absorption coefficient of the specimen for the wavelength of the analysis line of the element whose concentration is being corrected.

STCONC..Concentrations in the standards of all the elements whose concentrations are being determined, arranged in the same order as the data are input for the specimen.

STFC....The fluorescence corrections for the standards - computed the first time and then stored until termination of *PROBEDATA*.

STM.....A matrix containing element concentrations of the standards. The matrix has 20 columns (limiting the number of elements that can be included in any standard to 20) and a number of rows equal to the number of standards.

STMU....χ for the standard - i.e. the mass absorption coefficient of the standard for the wavelength of the analysis line of the element whose concentration is being corrected.

STMZ....A matrix containing atomic numbers of elements in the standards. The matrix has 20 columns and a number of rows equal to the number of standards.

X.......A list of all the atomic numbers of elements present in the specimen and all the standards, arranged (by *APLOADA*) in order of increasing atomic number.

XEA.....Assumed (or apparent) concentrations of elements present in the specimen which will not be corrected by the program (except by *AJST* or *CALC* subroutines).

XF......The slope of logarithmic equations fitted to Reed's (1965) curves for the D term of his fluorescence correction factor γ. Intermediate values of *XF* have been obtained by extrapolation. (Table 2).

XTRA....The number of elements present in the specimen whose concentrations were assumed.

YA......A list of atomic numbers of elements whose mass absorption coefficients were assembled from WS-1 by *APLOADA*. These correspond to wavelengths of K lines.

YB......A list of atomic numbers of elements whose mass absorption coefficients were assembled from SW-2 and WS-3 (by *APLOADB* and *APLOADC*). These correspond to wavelengths of L lines.

YC......A variable corresponding to the number of elements that appear in both *YA* and *YB*.

Z.......The atomic numbers of all the elements present in the specimen (analyzed and assumed) in the same order as *CONC*.

ZCOR....A vector containing the atomic number corrections - i.e. the factor by which the apparent concentration must be multiplied to take account of atomic number effects in both specimen and standard.

ZD......A vector containing the atomic numbers of assumed elements in the same order as *XEA*.

ZF......A variable depending on the difference in atomic number of two elements, and used in combination with columns 2-5 inclusive of matrix *FL* (Table 1) to determine whether or not fluorescence of one element by another will occur.

ZL......A list of atomic numbers corresponding to the code numbers 1 to 90 (Table 2).

ZSYM....A matrix of characters to give element symbols. The first column is filled by blanks, the second by the first letter of the element symbol and the third by the second letter of the element symbol. In the situation where the element symbol has only one letter, the second column is also left blank and the letter goes into the third column. The matrix may be set up as follows:

```
ZSYM←(92,3)⍴'  H HE LI BE B C..............  U'
```

KANSAS GEOLOGICAL SURVEY COMPUTER PROGRAM
THE UNIVERSITY OF KANSAS, LAWRENCE

PROGRAM ABSTRACT

Title (If subroutine state in title):

PROBEDATA (SUBROUTINES: READATA, MUCO, FLC, RND, APLOADA, APLOADB, APLOADC)

Date: January 1970

Author, organization: D.G.W. Smith and M.C. Tomlinson
University of Alberta

Direct inquiries to:

Name: Prof. D.G.W. Smith

Address: Dept. of Geology, University of Alberta
Edmonton 7, Alberta, Canada

Purpose/description: To correct data output by an electron microprobe for background, dead-time, absorption, fluorescence and atomic number effects and to manipulate corrected data to calculate structural formulae for minerals, concentrations of elements present but not analyzed, etc.

Mathematical method: An iterative procedure using the Heinrich-modified Philibert-expression for absorption correction, Reed fluorescence correction and Duncumb and Reed atomic number correction.

Restrictions, range: Elements with atomic number greater than 10 can be corrected. Intensities from M lines cannot be corrected.

Computer manufacturer: IBM

Model: System/360 Model 67

Programming language: APL

Memory required: 120,000 K

Approximate running time: variable - depending upon data corrected

Special peripheral equipment required: IBM remote terminal No. 2741 or 2740 or 1050

Remarks (special compilers or operating systems, required word lengths, number of successful runs, other machine versions, additional information useful for operation or modification of program) (1) A description of minor modifications which will permit some statistical evaluation of the input and output data may be obtained from the authors on request. (2) At the time of writing APL is only available (commercially) through IBM computers. Some universities are however running an APL system on other computers. (3) No modifications should be necessary to the listings to run the program at other centers. At the University of Alberta APL is run under the OS system and has in the past been run under the DOS system.

(continued from inside front cover)

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