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GEOCAPS, an interactive geochemical-data analysis program system in BASIC

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Abstract: GEOCAPS is an integrated interactive data-processing program system mainly for chemical analyses of rocks, minerals, and waters. The system is written in BASIC and HP-GL for Hewlett-Packard (HP) computers such as 200 series of HP-9000 making the best of the characteristics of interpreter language. The system comprises up to 13 programs: File creation, File edit, File copy (all for file management), Table print, Arithmetic calculation, Mean values, Correlation coefficients (for table listing), Histograms, X-Y diagrams, Piled X-Y diagrams, Triangular/Tetragonal diagrams, Hexa diagrams, and Key diagrams (for graphic output).

Main functions which characterize GEOCAPS are as follows: Data are selected for processing by specifying codes defined to classify samples. Total weight percentage of chemical-analysis data can be re-calculated into 100 percent. The data are able to be converted into molecular ratios or equivalents. Values of total Fe_2O_3 and total FeO are easily computed in both weight and mole from Fe_2O_3 and FeO. The CIPW normative calculation is possible and its result is treated together with other components. One of the most powerful functions of GEOCAPS is that interactive calculation among components can be performed by entering arithmetic expressions of components. The system flexibly responds to users' needs of various kinds and levels due to above functions.

1. Introduction

Geochemical studies are usually inductively carried out for finding new principles or evidences through calculations on a lot of chemical data. In most cases the geochemical data are transformed into atomic or molecular ratios, or equivalents. Total Fe_2O_3 and total FeO is computed from Fe_2O_3 and FeO. The CIPW normative calculation is necessary for silicate analyses of igneous rocks. Further, special diagrams are needed for presentation of geochemical data.

To date computer programs such as MULTIPLAN and dBASE-series have been released for numeric calculations. These tools designed for general purposes are, however, not always sufficient for geochemical studies although it is difficult to compare these systems critically. At least, calculations of geochemical data are much more complicated than usual ones, as mentioned in above paragraph. Therefore it is not

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efficient to apply ready-made programs for general use to geochemical data-processing even if they are managed to be combined with each other.

The authors planned to create an integrated system corresponding to the demands of researchers who study on chemical-analysis data of rocks, minerals, and waters. The basic ideas for GEOCAPS are as follows: First, the system must flexibly respond to various needs of researchers. Second, the system should be easily operated because geochemical data would be repeatedly processed with trial and error in the course of a study. Third, the system should equip powerful graphic functions that are essential for scientific discussion and presentation (YOSHII and SATO, 1983 a, 1983 b).

In 1974 the study was started to make an interactive program system for the Hewlett-Packard (HP) personal computer HP-9820 A to process petrochemical data. Since 1980 the authors have modified these programs for the computer HP-9845 T and then 9836 A, 200-series of the HP-9000, to apply the system to many kinds of chemical-analysis data. The HP-devices can satisfy the authors demands because they run on an interpreter BASIC and equips exellent graphic commands named HP-GL.

How to transfer data in the HP-computer to other devices have been established by KOUDA (1983, 1984) with a special connecting cable through RS-232 C. Owing to this, table listing is possible with remote printers. Further, GEOCAPS data can be sent to other computers for data-processing in other program systems (YOSHII, 1986).

Table 1 Programs and their main functions.

Programs	Main Functions					
	Sort Data	Select Data by Codes	Arithmetic Calculation	Print Tables	Graphics Dots/Lines	
*File Management						
File Creation (No. 1)						
File Edit (No. 2)	○			○		
File Copy (No. 3)	○	○				
*Table Listing						
Table Print (No. 4)	○	○	○	○		
Arithmetic Calculation (No. 5)	○	○	○	○		
Mean Values (No. 6)	○	○	○	○		
Correlation Coefficients (No. 7)	○	○	○	○		
*Graphic Output						
Histograms (No. 8)	○	○	○			○
X-Y Diagrams/Maps (No. 9)	○	○	○		○	○
Piled X-Y Diagrams (No. 10)	○	○	○		○	
Triangular/Tetragonal D. (No. 11)	○	○	○		○	○
Hexa Diagrams (No. 12)	○	○	○			○
Key Diagrams (No. 13)	○	○	○		○	○

Note: 1. ○: able.
2. CIPW Normative Calculation is able in Program Nos. 4-11 of N-Series.
3. Key Diagrams is only in W-Series.

2. Structure of the system

GEOCAPS is made up of three series of programs in accordance with types of data : the N-series, G-series, and W-series. The N-series mainly treats silicate-analysis data of igneous rocks with the CIPW normative calculation. The G-series processes general geochemical data. This series is useful also for general numerical data of other fields. The W-series is for water analysis data. Each series comprises up to 13 programs and a menu program. They are as follows :

Program menu
Programs for file management
  File Creation (No. 1)
  File edit (No. 2)
  File copy (No. 3)
Programs for table listing
  Table print (No. 4)
  Arithmetic calculation (No. 5)
  Mean values (No. 6)
  Correlation coefficients (No. 7)
Programs for graphic output
  Histograms (No. 8)
  X-Y diagrams/maps (No. 9)
  Piled X-Y diagrams (No. 10)
  Triangular/tetragonal diagrams (No. 11)
  Hexa diagrams (No. 12)

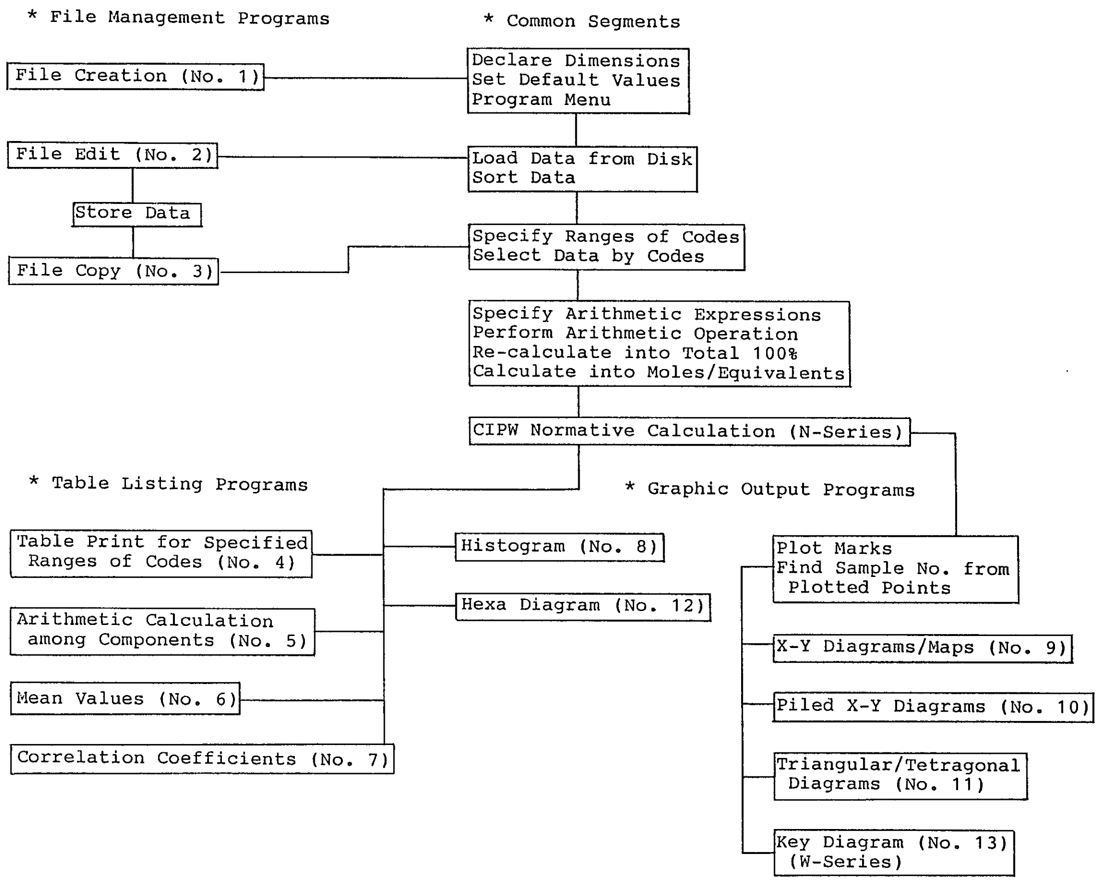

Fig. 1 Diagram showing the assemblage of segments for main functions of each program.

Table 2 An example of the data table with the CIPW normative calculation and arithmetic calculations among components.

Chemical-Analysis Data of Igneous Rocks
WITH Normative Calculation.

Serial	6	17	32	36	38	40	90	101	117	128
No.	JGb-1	ON2040G	JB-3	JB-1	ON437MI	JB-2	JA-1	ON907KA	JG-1	JR-1
Code	RGBRSTD...	VBAS......	RBASSTD...	RBASSTD...	VBASAO....	RBASSTD...	RANDSTD...	VANDH.....	RGRNSTD...	RRHYSTD...
SiO2	43.44	49.09	51.04	52.17	53.01	53.20	64.06	67.31	72.30	75.41
TiO2	1.62	.60	1.45	1.34	.61	1.19	.87	.39	.26	.10
Al2O3	17.66	22.45	16.89	14.53	14.83	14.67	14.98	15.23	14.20	12.89
Fe2O3	4.89	2.59	3.10	2.28	5.35	3.13	2.42	.19	.39	.40
FeO	9.24	4.78	7.90	6.00	9.98	10.09	4.08	2.67	1.63	.50
MnO	.17	.13	.16	.16	-	.20	.15	.06	.06	.10
MgO	7.83	6.00	5.20	7.73	3.83	4.66	1.61	1.23	.74	.09
CaO	11.98	7.90	9.86	9.29	9.97	9.89	5.68	3.94	2.18	.63
Na2O	1.23	2.14	2.82	2.79	1.76	2.03	3.86	3.33	3.39	4.10
K2O	.26	2.65	.80	1.42	.46	.43	.82	2.37	3.95	4.44
P2O5	.05	.10	.29	.26	.32	.10	.16	.19	.10	.02
H2O+	1.23	1.68	.20	.95	.01	.31	.80	2.10	.07	1.05
H2O-	.04	.88	.03	1.02	.01	.07	.26	.32	.48	.13
Others	.....	.....	.....	.18	.....	.31	.....	.....	.07	.....
Total	99.64	100.99	99.74	100.12	100.14	100.28	99.75	99.33	99.82	99.86
T.FeO/MgO	1.74	1.19	2.06	1.04	3.86	2.77	3.89	2.31	2.68	9.55
NA2O+K2O	1.49	4.79	3.62	4.21	2.22	2.46	4.68	5.70	7.34	8.54
A	.181	.174	.131	.097	.146	.126	.091	.072	.045	.016
C	.214	.141	.176	.166	.178	.176	.101	.070	.039	.011
F	.325	.217	.241	.278	.234	.259	.099	.069	.042	.011
Q	-	-	2.47	1.16	12.46	9.41	23.67	27.21	30.90	32.87
C	-	1.94	-	-	-	-	-	.48	.62	.24
or	1.54	15.66	4.73	8.39	2.72	2.54	4.85	14.01	23.34	26.24
ab	10.41	18.11	23.86	23.61	14.89	17.18	32.66	28.18	28.68	34.69
an	41.90	38.54	31.06	22.93	31.21	29.65	21.13	18.30	10.16	2.99
wo-di	7.19	-	6.66	8.96	6.75	7.83	2.51	-	-	-
en-di	4.40	-	3.65	6.02	2.87	3.49	1.19	-	-	-
fs-di	2.38	-	2.77	2.26	3.89	4.31	1.29	-	-	-
en-hy	7.99	10.39	9.30	13.23	6.66	8.12	2.82	3.06	1.84	.22
fs-hy	4.33	4.09	7.07	4.96	9.01	10.03	3.05	4.21	2.35	.61
fo-ol	4.99	3.19	-	-	-	-	-	-	-	-
fa-ol	2.98	1.39	-	-	-	-	-	-	-	-
mt	7.09	3.75	4.49	3.31	7.76	4.54	3.51	.28	.57	.58
il	3.08	1.14	2.75	2.54	1.16	2.26	1.65	.74	.49	.19
ap	.12	.23	.67	.60	.74	.23	.37	.44	.23	.05
Others	1.27	2.56	.23	2.15	.02	.69	1.06	2.42	.62	1.18
Total	99.64	100.99	99.74	100.12	100.14	100.28	99.75	99.33	99.82	99.86
D.I.	11.94	33.77	31.06	33.16	30.07	29.13	61.18	69.39	82.93	93.80
Or Mol%	2.8	21.3	7.7	14.9	5.5	5.0	8.0	22.5	36.5	39.7
Ab	20.3	26.2	41.4	44.4	31.8	36.1	57.1	48.0	47.6	55.7
An	76.9	52.5	50.9	40.7	62.8	58.8	34.9	29.4	15.9	4.5

Data are Sorted on SiO2 Values in Ascending Order.
Processed by GEOCAPS-T using YHP9845T.
Ouput to Brother HR-15 Printer through RS-232C.

Note 1) Arithmetic calculations are added below the analytical data and below the D.I.
2) Serial Nos. 17, 38, and 101 from Ono (1962), others from Ando (1983) *et al.*

Key diagrams (No. 13) (W-series only)

Main functions that characterize the system are shown in Table 1. The programs are made up of 7,000 steps which comprise about 60 segments. The assemblage of segments for main functions of each program is shown in Fig. 1.

A set of users' files for GEOCAPS consist of the index-file, component-file, data-file, and code-file. The index-file keeps names of the component-file and data-file, maximum and current numbers of samples and components, data-type, and others. The component-file contains names of components and their atomic or molecular weights. The data-file has data of analytical samples: sample-numbers, codes, and values of each component. The code-file stores up to 20 sets of ranges of codes by which the user select data for processing.

2.1 File management

2.1.1 File creation (Program No. 1)

This program is used to define the user's files. Components are usually entered from the keyboard. Atomic or molecular weights for the chemical components are automatically calculated and stored into the component-file. Another component-file can be quoted instead of entering from the keyboard (Yoshii, 1983 a).

2.1.2 File edit (Program No. 2)

This program is for entering, correcting, printing, sorting, reordering, and storing data. Data are usually entered from the keyboard. The data of coordinates, latitudes and longitudes, can be entered from a digitizer. Data can be edited on samples and components: Samples are sorted, reordered, and deleted. Components are reordered, added, and deleted (Yoshii, 1983 c). When data are partly lacking, the value of "no-data" is defined to be 9.0 E + 63. Data of this value are omitted in processing.

Table 3 An example of the table resulted from arithmetic calculations among components to get ion ratios of rhodonite.

Serial	No.	Code	T.Anion	15/Tot.	Si	Al	Fe'''	Fe''	Mn	Mg	Ca
29	IN.CHIKLA.	RRDN...DHZ	2.301	6.520	4.933	.035	-	.087	4.645	.089	.262
30	J.TAGUCHI.	RRDN...M64	2.275	6.595	4.875	.106	.033	.140	4.634	.087	.180
31	J.ZOMEKI..	RRDN...M64	2.263	6.629	4.852	.121	.022	.054	4.595	.127	.305
33	J.CHIZU...	RRDN...M64	2.278	6.583	4.711	.276	-	.204	4.431	.023	.505
34	NZ.ARROW..	RRDN...DHZ	2.322	6.459	4.990	.009	.009	.134	4.336	.147	.375
35	J.TAMAIWA.	RRDN...M64	2.322	6.461	4.915	.108	.063	.190	4.299	.011	.414
36	J.AKIMOTO.	RRDN...M64	2.289	6.552	4.933	.066	.010	.025	4.356	.041	.601
37	J.KIURA...	RRDN...M64	2.245	6.681	4.894	.125	-	.102	4.393	.123	.407
42	J.YOSHIDA.	RRDN...M64	2.340	6.410	4.936	.124	.039	.027	4.161	.068	.626
43	J.NODATAMA	RRDNBaOY67	2.302	6.515	5.057	.023	.022	.044	4.222	.002	.551
45	07-9018R..	RRDN...Y78	2.331	6.435	5.001	.019	-	.038	4.161	.246	.524
46	J.HORIGOSH	RRDN...M64	2.281	6.577	4.902	.041	.040	.200	4.247	.023	.605
54	J.YAMATO..	RRDN...M64	2.221	6.753	4.835	.030	.019	.025	4.330	.270	.630
55	07-706R...	RRDN...Y78	2.335	6.423	4.898	.115	.051	.016	4.118	.449	.371
	Number of Samples		14	14	14	14	14	14	14	14	14
	Mean Value		2.293	6.542	4.910	.086	.022	.092	4.352	.122	.454
	Standard Deviation		.035	.102	.082	.071	.021	.070	.174	.125	.145
	Maximum Value		2.340	6.753	5.057	.276	.063	.204	4.645	.449	.630
	Minimum Value		2.221	6.410	4.711	.009	-	.016	4.118	.002	.180

Note: Serial Nos. 29, 34 from Deer *et al.*; 30-33, 35-42, 46-54 from Momoi(1964); 43 from Yoshimura (1967); 45, 55 from Yoshii (1978).

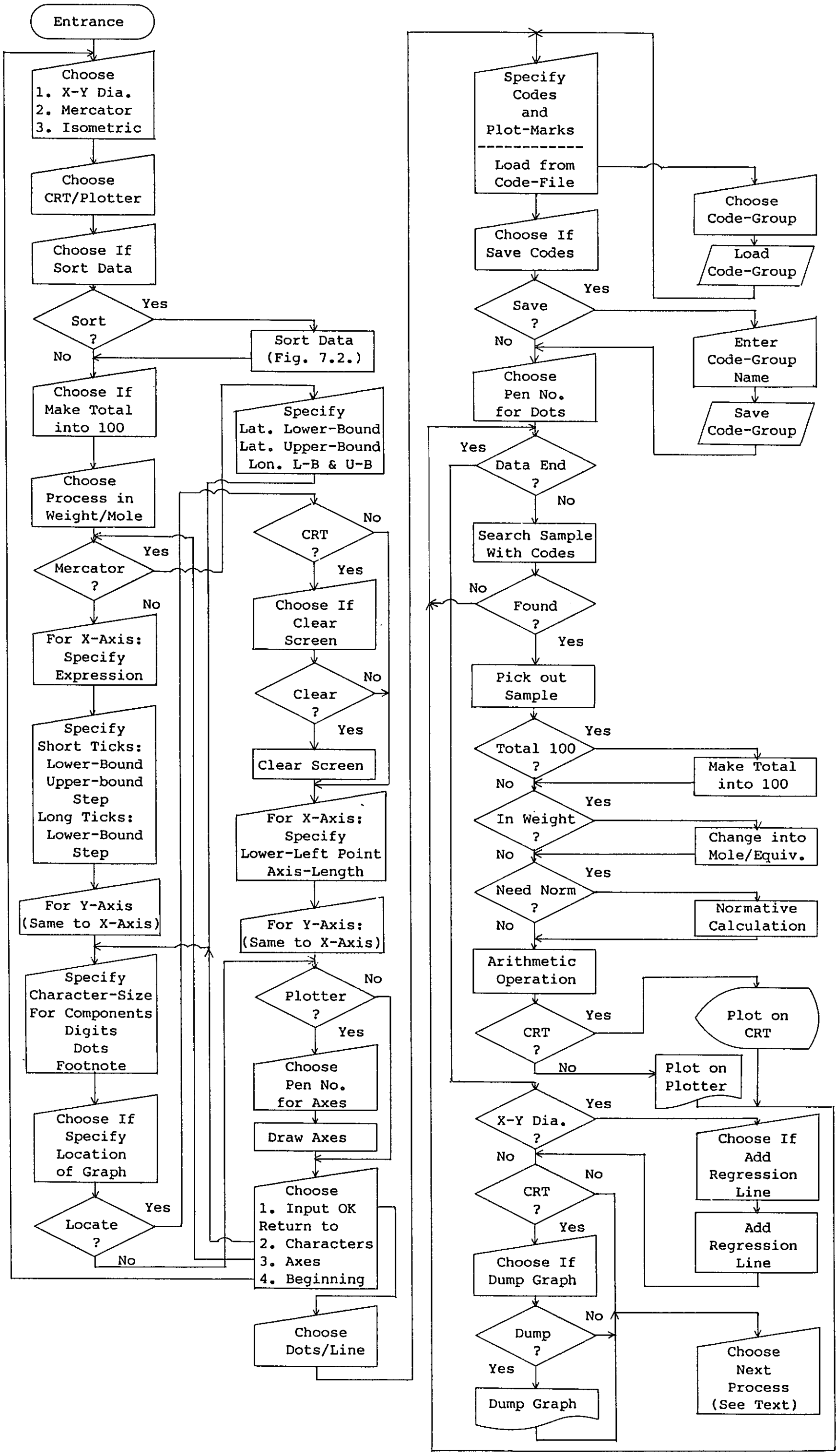

Fig. 2 Flowchart for plotting X-Y diagrams and maps.

2.1.3 File copy (Program No. 3)

This program copies data into another disk-file. Data are selected by the specified ranges of codes in the same way as the following data-processing programs. This program is useful for making sub-files to carry out efficient processing.

2.2 Table listing

2.2.1 Table print for specified codes (Program No. 4)

This program prints samples selected by specified ranges of codes. The samples are arranged in columns on a table. In the N-series, results of the CIPW normative calculation are attached to the analytical data. Results of arithmetic calculations among components can be added. Up to 15 arithmetic expressions are acceptable. An example of the table with CIPW normative calculation is shown in Table 2.

2.2.2 Arithmetic calculation among components (Program No. 5)

This program tabulates computed values of total 15 arithmetic expressions of components. Samples are arranged in rows on a table. Values of maximum, minimum, mean, and standard deviation are added to each component. An example is given in Table 3.

2.2.3 Mean values (Program No. 6)

This program calculates maximum, minimum, and mean values, and standard deviations for a specified range of components and computed values of an arithmetic expression. The results are listed on a table.

2.2.4 Correlation coefficients (Program No. 7)

This program computes correlation coefficients for a pair of specified ranges of consecutive components, or a pair of computed values of components. The results are listed on a table.

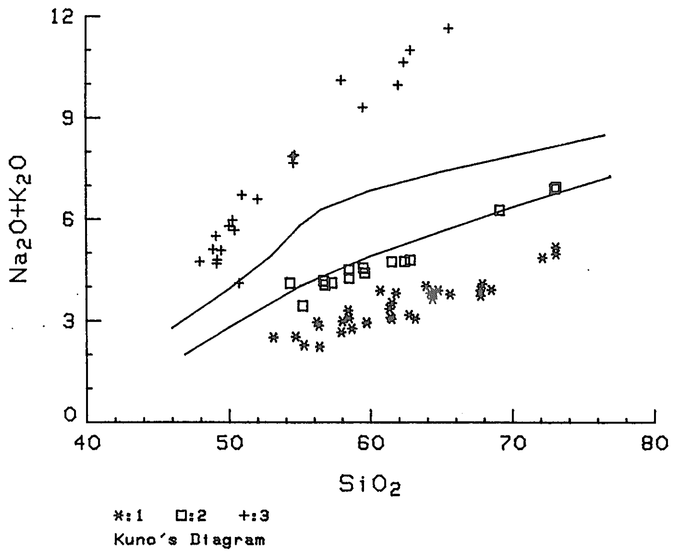

Fig. 3 Kuno's diagram, an example of the X-Y correlation diagram.
1: Osore-yama Volcano (Togashi, 1977). 2: Asama Volcano (Okamoto, 1979).
3: Jeju Island (Lee *et al.*, 1982).

2.3 Graphic output

2.3.1 Histograms (Program No. 8)

This program draws histograms for the computed values from an arithmetic expression of components. Frequency is calculated on absolute numbers or percentage by choice. Number of processed samples, the frequency against each step, the mean value, and the standard deviation are printed.

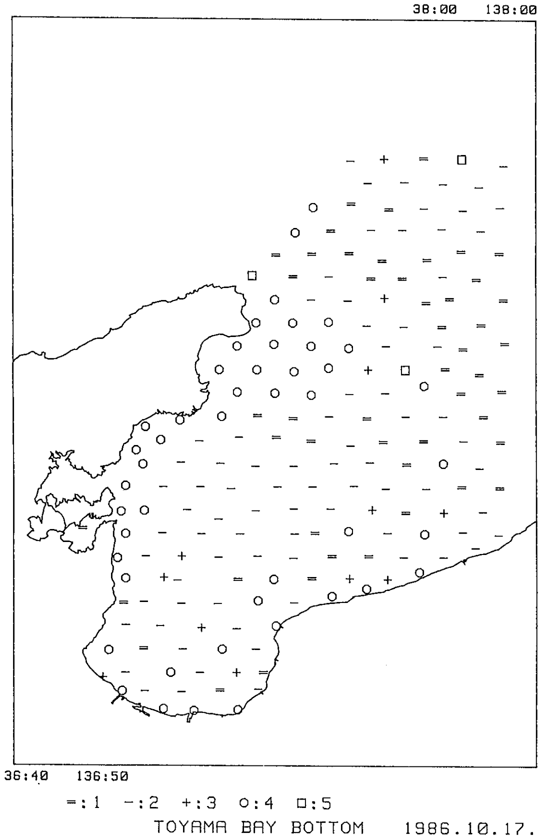

Fig. 4 Distribution of bottom sediments in Toyama Bay, an example of the Mercator map.
Data are from ARITA *et al.* (1979).
1: Clay. 2: Silt. 3: Sand, silt, and clay. 4: Clayey to fine sand. 5: Rock basement.

2.3.2 X-Y diagrams and maps (Program No. 9)

This program plots X-Y diagrams for computed values. A regression line can be added, if necessary. Number of processed samples and correlation coefficient are printed. The Mercator projection maps are also drawn from the given ranges of latitude and longitude if the location data exist in the component-file. The flowchart of this program is shown in Fig. 2.

As an example of the X-Y diagram the Kuno's diagram (KUNO, 1965) is given in Fig. 3. The authors have prepared the data for boundary lines of the diagram so that the user can make the diagram in any range of values (YOSHII and SATO, 1984 c). An example of a distribution map is shown in Fig. 4. Data for the coast line are previously entered into a data-file from a map with a digitizer.

2.3.3 Piled X-Y diagrams (Program No. 10)

This program is for correlation diagrams between the specified computed value on X-axis and other maximum 15 computed values on Y-axis. A regression line can be added to each pair. Numbers of processed samples and correlation coefficients are printed. Harker's diagrams are plotted with this program. An example of the piled X-Y diagram is given in Fig. 5.

2.3.4 Triangular and tetragonal diagrams (Program No. 11)

This program draws triangular, or tetragonal diagrams. End members are given as arithmetic expressions among components. The tetragonal diagrams are originated by ARAMAKI *et al.* (1970, 1972). Geometry for plotting a tetragonal diagram in this program is shown

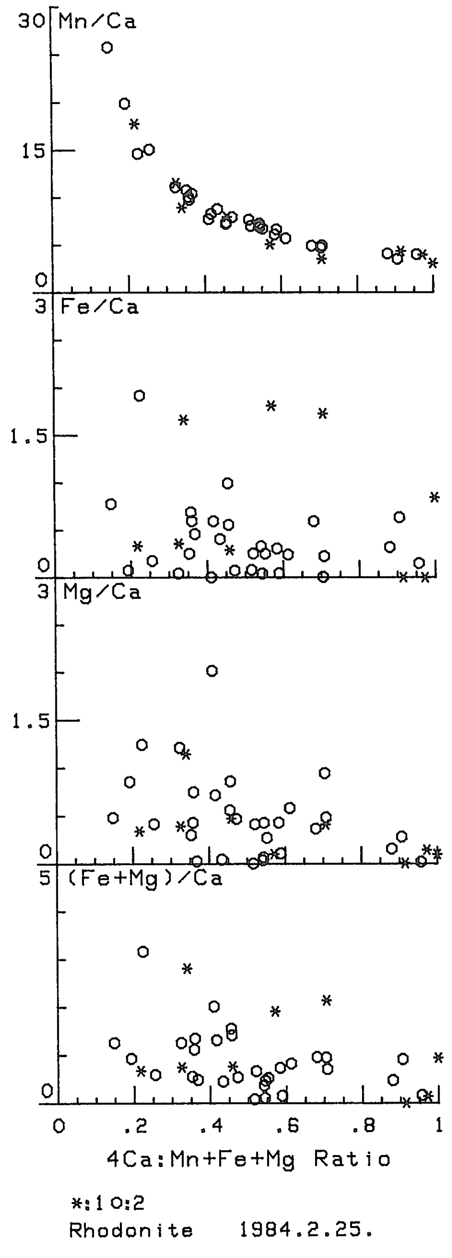

Fig. 5 Correlation between Ca and metal ions in rhodonite, an example of the piled X-Y correlation diagram. Data are from DEER *et al.* (1963), MOMOI (1964), YOSHII (1978), and YOSHIMURA (1967).

by SATO and YOSHII (1981). An example of the tetragonal diagram is given in Fig. 6.

2.3.5 Hexa diagrams (Program No. 12)

This program is for hexa diagrams for a set of six computed values from arithmetic expressions of components. Data are processed in atomic or molecular ratios, or in equivalents. In case of water-analysis data, total of cations must be balanced with that of anions. Therefore samples will be omitted in processing in case that the difference of the totals is larger than a specified threshold. Although hexa diagrams are originally for water-analysis data, they can be applied to data of other fields for comparing the compositions of the data with patterns. An example of the diagram is shown in Fig. 7.

2.3.6 Key diagrams (Program No. 13)

This program plots ratios among four computed values. This diagram is only for water-analysis data. Processing is always performed in equivalent. Data will be omitted in processing in case that the difference of total of cations and that of anions is larger than a specified threshold. An example of the diagram is given in Fig. 8.

3. Common functions among programs

The above mentioned programs have several common functions which characterize the GEOCAPS. Main functions are shown in Fig. 1. They are described in the following sections.

3.1 Searching data by code

Data in a file can be picked out for processing by the classification code which is put onto every sample. The

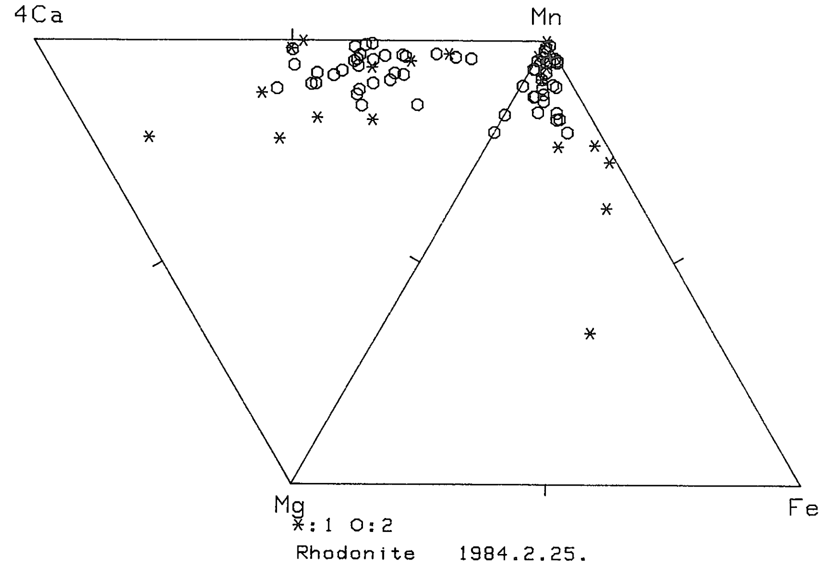

Fig. 6 Ca and metal ratios in rhodonite, an example of the tetragonal diagram. Data are the same to Fig. 6.

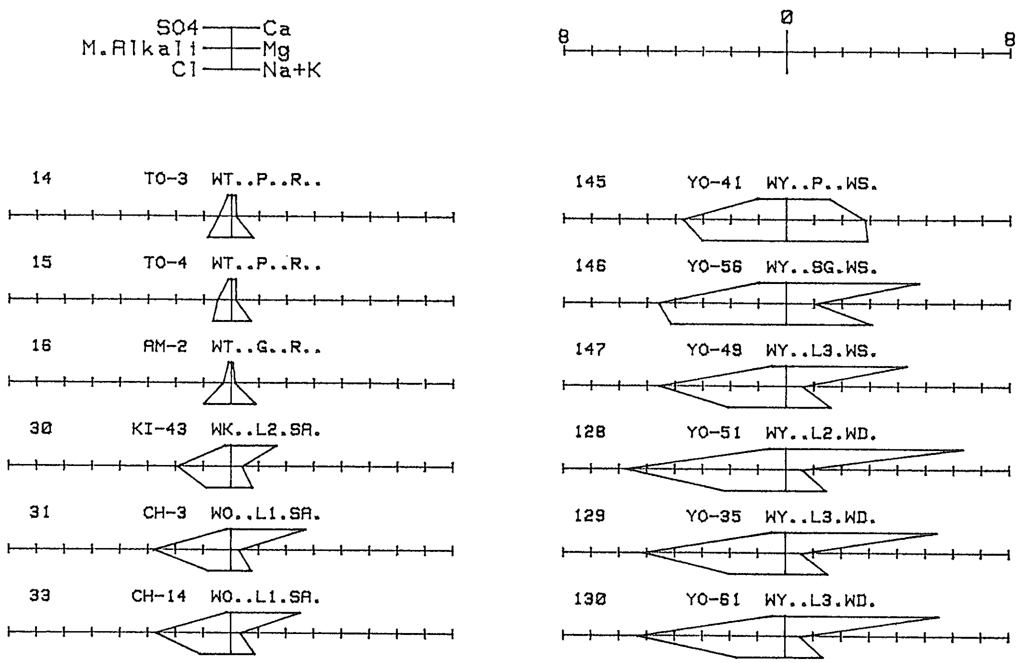

Fig. 7 Hexa diagrams applied to water analysis.
From Goto's unpublished data.
14–16: River in Tokunoshima Island. 30–33: Spring in Kikai and Okinoerabu Islands. 145–147: Shallow well in Yoron Island. 128–130: Deep well in Yoron Island.

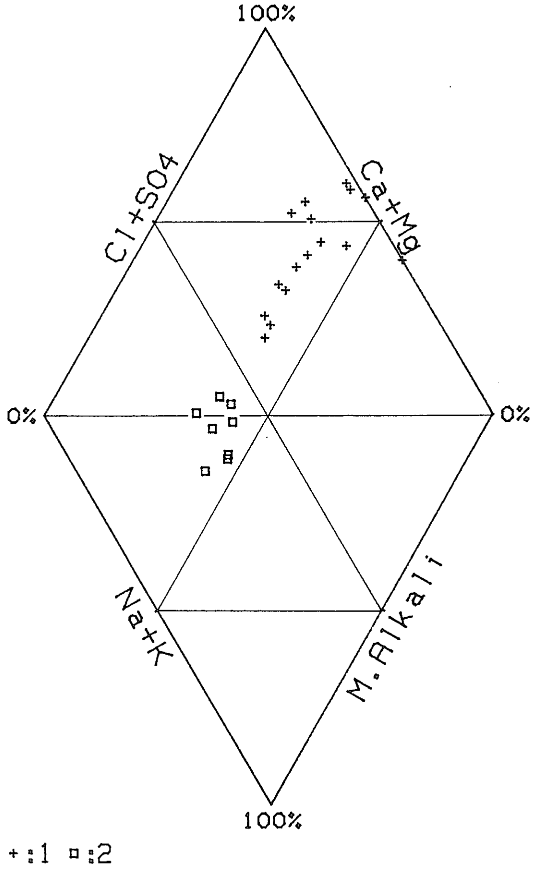

Fig. 8 River and well waters, an example of the key diagram.
From Goto's unpublished data.
1 : River. 2 : Well.

code is composed of 10 characters. They are divided into four sub-codes. The first sub-code is one character and the rests three, as like,

ABBBCCCDDD

where A, B, C, and D stand for each sub-code. The user defines each sub-code to classify his data on any four independent factors, such as geologic regions, age, kinds of samples, and so on.

In the course of data-processing, the user specifies the range of each sub-code. Logically each range of sub-codes is connected with the "AND" operator of the Boolean expression. Up to nine sets of ranges of sub-codes can be specified at one time. The sets are connected with the "OR". Twenty back-trace data are able to be stored in the code-file for convenience of repeated jobs on the same group of samples (Yoshii, 1980).

Program steps of searching data with specified codes are shown in Appendix 1.

3.2 Arithmetic calculations of components

Interactive algebraic operations are applied among components, normative minerals, and D.I. (differentiation index) in every data-processing program. The operations are performed with the operation-code method reported by the authors (Yoshii, 1984 a, 1985 ; Yoshii and Sato, 1983 a, 1984 b). All the user has to do is to give arithmetic expressions of components from the keyboard.

Rules for the expressions are nearly the same to usual algebraic ones. The multiplication symbol "*" can be omitted in case that a constant precedes a component or the opening parenthesis "(". Multiplex parentheses and logarithmic functions, log and ln, can be used.

When an expression

Total=100MgO/(MgO+T.FeO);MgO%

is entered from the keyboard, for example, the characters are broken down into constants, components, mathematic symbols, delimiters, and characters for the label. Characters on the left-side of the delimiter "=" is the component that the result from the calculation is entered.

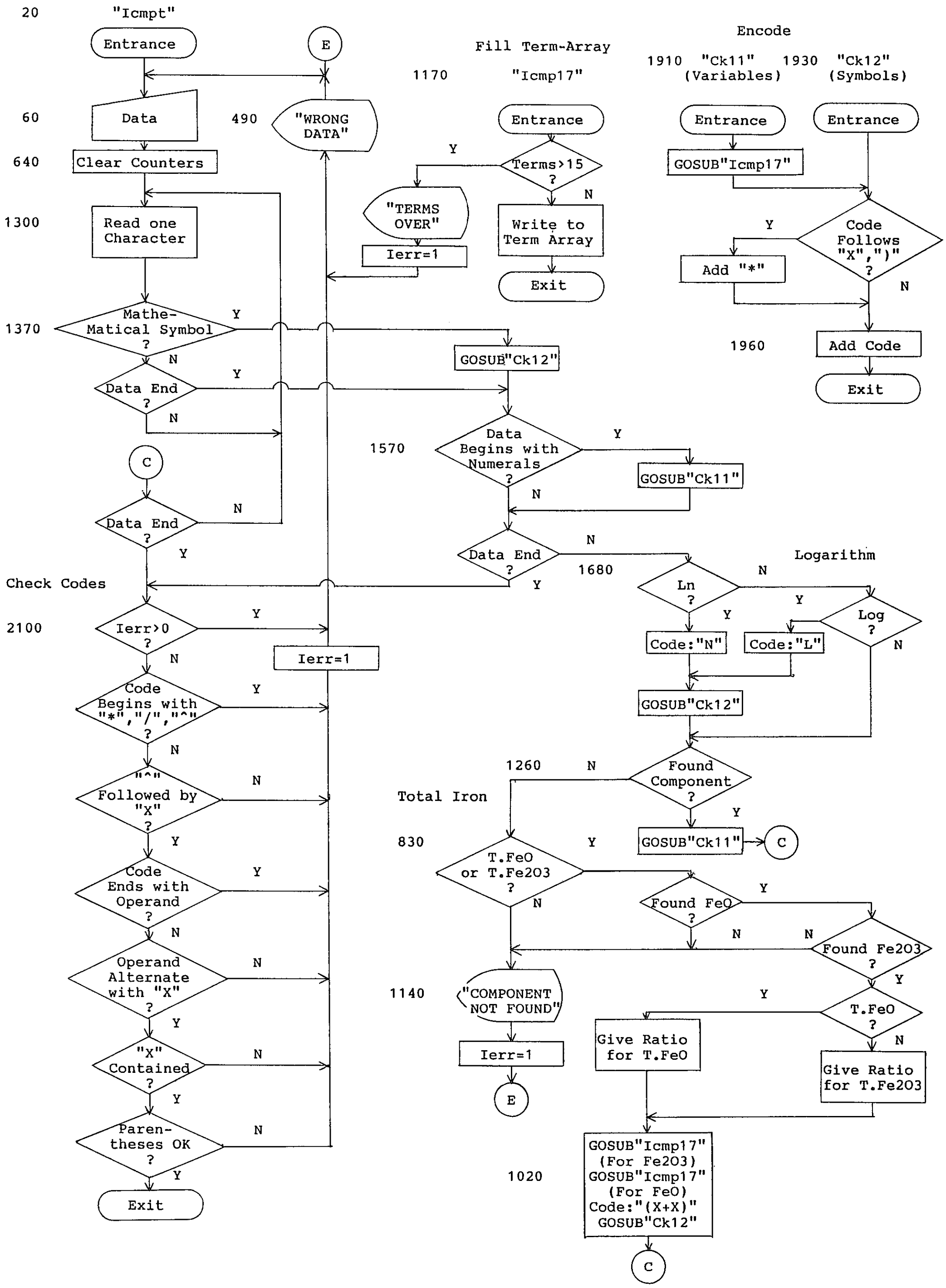

Fig. 9 Flow of operations to build an operation-code for the entered expression of components.

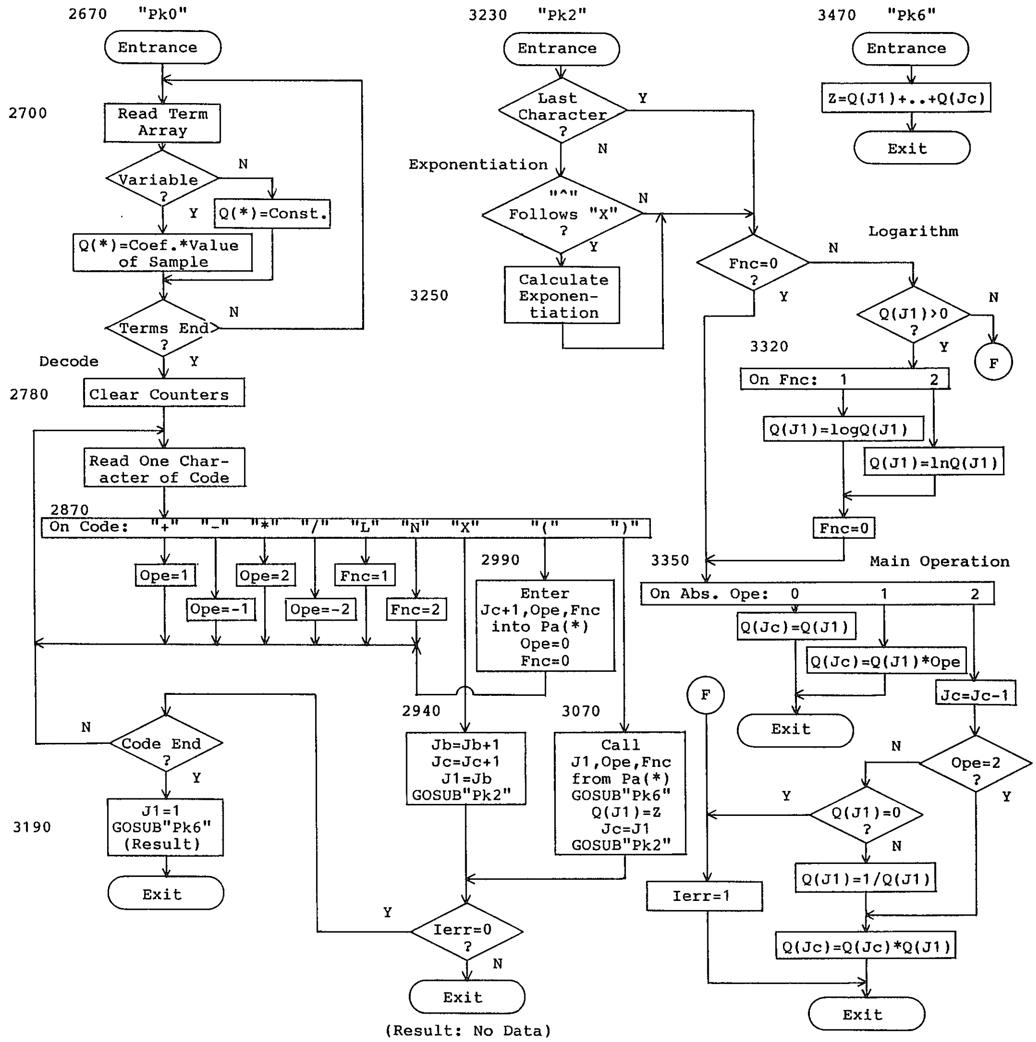

Fig. 10 Flow of operations to execute calculations along the operation-code.

In accordance with the given expression, the operation-code

X∗X/(X + (X + X))

is internally built up. In above case the operation-code for T.FeO that stands for total FeO is "(X + X)" because T.FeO is composed of two components, Fe_2O_3 and FeO. Specified components are entered into an array B1(∗) as the ordinal number of the components in the component-file. Values of coefficient or constant are stored into B2(∗). The arrays are named the term arrays. In this paper the symbol "(∗)" collectively expresses an array. Finally the operation-code is checked if it is mathematically valid, or not. The flowchart of these steps are given in Fig. 9. The program list is in Appendix 2.1.

In the course of data processing, data of a selected sample are moved into the calculation array Q(∗). Calculations are performed according to the operation-code. The flow of the calculation is shown in Fig. 10. The program list is in Appendix 2.2. In the above example the result is entered into the component "Total". The characters "MgO %" will appear on tables or diagrams as the label instead of the given expression.

3.3 The CIPW normative calculation

The CIPW normative calculation is performed in data-processing programs of the N-series. Cr_2O_3 and NiO are acceptable. Although it is basically after CROSS *et al.* (1902), the calculation is slightly modified. Namely, the molecular weight of FeO is calculated as the weighted average of FeO, MnO, and NiO. In this way total weight-percentage of normative minerals can correspond to that of analytical data (YOSHII and HIRANO, 1977 ; YOSHII, 1984 b).

The normative minerals and D.I. are internally generated, and their values can be treated together with other components. In GEOCAPS normative corundum is designated as "C′" for distinguishing from carbon (C).

3.4 Other functions

Following functions can be applied :

1) Data are sorted on sample-numbers in ascending order, on sub-codes in ascending order, and on components in ascending/descending order. In the latter two cases, two keys can be specified (YOSHII, 1983 b).

2) The data are re-calculated into their total 100 in case that the component "Total" or "Sum" exsists in the component-file. In the N-series the values from SiO_2 through P_2O_5 are totalized.

3) The selected data are converted into atomic or molecular ratios, or equivalents in case of water-analysis data.

4) In posting programs, such as X-Y diagrams, piled X-Y diagrams, triangular/tetragonal diagrams, and key diagrams, any capital letters on the keyboard are used as plot-marks. Broken lines can also be used in the programs except piled X-Y diagrams. The sample-number and code of each posting point on the CRT or the plotter are able to be found using a digitizing operation.

4. An example of application

Examples of applications of GEOCAPS to petrochemistry, mineralogy, and hydrology are shown by YOSHII and SATO (1984 b). An example of the application to mineralogy is explained in the following lines :

Experimental formulas of rhodonite of which ideal formula is $CaMn_4Si_5O_{15}$ can be calculated with the program No. 5. The data are from DEER *et al.* (1963), MOMOI (1964), YOSHII (1978), and YOSHIMURA (1967).

The data are processed in molecular ratios. Total nine arithmetic expressions are specified in order. Steps of entering the expressions are as follows :

1) Entering total of anions into the component "Total". The label of the arithmetic expression is "T. Anion".

```
TOTAL = 2SIO2 + 3AL2O3
  + 3FE2O3 + FEO + MNO + MGO
  + CAO ; T. Anion
```

2) Entering ratio of 15 oxygens against total anions into the "Total" again. The label for the expression is "15/Tot.".

```
TOTAL = 15/TOTAL ; 15/Tot.
```

3) Each cation ratio is given on the basis of 15 oxygens. The expressions are as follows :

TOTAL*SIO2 ; Si
TOTAL*2AL2O3 ; Al
TOTAL*2FE2O3 ; Fe'''
TOTAL*FEO ; Fe''
TOTAL*MNO ; Mn
TOTAL*MGO ; Mg
TOTAL*CAO ; Ca

Results of the calculations are listed in Table 3. Data are sorted on MnO in descending order. The results of the steps 1 through 2 can be omitted in the table, if necessary.

5. Conclusion

In most cases computation of data in scientific fields are performed with some fixed formulas. But in geoscientific studies such formulas or rules are inductively searched out of the results from data processing with trial and error. Therefore interactive processing is inevitable in these studies.

GEOCAPS provides special functions considering the characteristics of geochemical data. In the course of processing, data are automatically re-calculated into atomic or molecular ratios, or equivalents, if necessary. Results of the CIPW normative calculation can be used for further processing.

One of the most striking functions of GEOCAPS is arithmetic calculation among components without modifying any steps of programs. This function plays the most important role in data processing because the system is able to respond flexibly to the users' needs of various levels. Researchers can carry out many kinds of calculations only by entering arithmetic expressions of components.

Other important points of GEOCAPS are : First, the authors make the programs in the interpreter BASIC which is one of the most popular languages. Therefore the system can easily modified at any time needed, even temporarily, in accordance with the users' needs. Second, the authors picked out the HP-computers because they have excellent and powerful graphic functions named HP-GL. In fact HP-GL have recently been adopted in many plotters.

GEOCAPS has been grown up to a total system for geochemical purposes. To date a lot of papers have been published by using this data-processing system by many researchers. This proves that the system can fully contribute to the studies of geoscientific fields.

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BASIC による対話型地球化学データ処理プログラムシステム GEOCAPS

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要　旨

GEOCAPS は主として岩石・鉱物・水の化学分析データの計算処理システムである．言語はヒューレットパッカード社の BASIC 及び HP-GL で書かれ，HP-9000 型 200 シリーズ計算機などの特徴を最大限利用できる．

システムは，1）新規ファイルの生成，2）データの入力・編集，3）ファイル内容の編集，4）数表の印刷，5）成分同士の計算，6）平均値・標準偏差の計算，7）相関係数の計算，8）度数分布図，9）相関図・分布図，10）積層型相関図，11）三角図・四面体図，12）ヘキサダイアグラム，13）キーダイアグラム，の各プログラムから構成される．

このシステムの特徴は，データ処理の過程で次の処理が容易に実行できる点である．1）利用者が定義しデータに付けた分類コードによるデータの検索及び処理．2）化学分析値合計値の 100% への再計算・モル比への換算・Fe_2O_3 及び FeO から全 Fe_2O_3 及び全 FeO への変換．3）CIPW ノルム計算の結果と他の成分の値との対等な処理．4）成分名を演算式の形で入力すれば，その算式に従った多成分間の計算が実現．以上の諸機能によって，GEOCAPS は利用者の多岐にわたる要求に，柔軟に対応できる仕組になっている．

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Appendix

1. Program List for Searching Data with Ranges of Specified Codes

Variables: Istart--lower bound of the serial-number. Istop--upper bound of the serial number. Cd$(*)--a specified code. Cd$(*)[1,1], Cd$(*)[2,4], Cd$(*)[5,7], and Cd$(*)[8]--sub-codes. No$(N(I),2)--the code of a sample. The symbol "(*)" collectively expresses an array.

```
700 Seld0:  ! [SD16] == SELECTNG DATA ON CODES (NGW) 83824
    ----
770 Seld:FOR I=Istart TO Istop
780     Z$=TRIM$(No$(N(I),1))
790     IF Z$[1,1]="-" THEN Seld3!  Samples of which 1st character of
serial No. is omitted in the data-processing.
800     Cd$(1)=No$(N(I),2)[1,1]!  1st sub-code.
810     Cd$(2)=No$(N(I),2)[2,4]!  2nd sub-code.
820     Cd$(3)=No$(N(I),2)[5,7]!  3rd sub-code.
830     Cd$(4)=No$(N(I),2)[8]!  4th sub-code.
840     FOR I0=1 TO 9
850       IF C0$(I0)="" THEN Seld3
860       FOR J0=1 TO 4
870         IF Cd$(J0)<C1$(I0,J0,1) OR Cd$(J0)>C1$(I0,J0,2) THEN Seld2
880       NEXT J0
890       GOTO Pick
900 Seld2:NEXT I0
910     GOTO Seld3
920 Pick: GOSUB Norl!  To data-processing.
930     GOSUB Process
940 Seld3: NEXT I
950    RETURN
960 Joint: END
```

2. Program List for Arithmetic Calculations

This segment is divided into two parts. The one is for interpretative analytical operations for given expressions of components. The other is for performing calculations with operation-code.

2.1. Building an operation-code from entered expressions of components

These steps are divided into two parts. Lines 10 through 2090 are for building the operation-code. Lines 2100-2660 are for checking whether the given expression is mathematically correct, or not.

Variables: Nc$(*)--Componets in the component-file. Cmp$(*)--Specified expressions. X$(*)--Operation-code. B1(*)--Component-number. B2(*)--Coefficient or constant. B1(*) and B2(*) are term arrays.

```
10 Entpro:   ! [IK67]=[IK26]+[PK16] (NGW) 85621
20 Icmpt:  ! [IK26] = INPUT 85621
30     Q$=""
40     La$=Cmp$(H4)
50     PRINT "Comp: ";La$;" ";
60     INPUT "Component ($80, up to 15-Terms, 5-fold Parentheses)",La$
70     GOSUB Icmp2
80     IF Ierr THEN RETURN
90     Cmp$(H4)=Q0$
100    PRINT Q0$
110    PRINT
120    Be(H4)=0
130    GOSUB Rcmp9
140    IF Z0 THEN!  When the delimiter "=" is found, the component on the
left side of "=" should be the component into which the result of
calculation is entered.
150      Q0$=La$[1,Z0-1]
160      GOSUB Icmp9
170      Q$=Q0$
180      GOSUB Scmp!  To make sure the component to accept the result
exits.
190      IF J0>Sc(4) THEN
200        GOSUB Icmp131
210        GOTO Icmpt
220      END IF
230      Be(H4)=J0
240      GOSUB Beep2
250      PRINT "Enter: ";Cmp$(H4);CHR$(130)&" into "&CHR$(128);Nc$(J0)
260      PRINT
270      PRINT "** You Must Memorize that the Data of ";Nc$(J0);" Will be
Changed."
280      PRINT "** Contents of the File will be Changed if You Record the
Data!"
290      Cmp$(H4)=Q$&"="&Cmp$(H4)
300    END IF
310    IF Z THEN
320      PRINT "Label:  ";TRIM$(La$[Z+1])
330      Cmp$(H4)=Cmp$(H4)&TRIM$(La$[Z])
340    END IF
350    PRINT
360    PRINTER IS Prn2
370 Picmpi:IMAGE #,2D,2X,10A,K,10X
380    PRINT "#";H4;Cmp$(H4);" ---- ";"FC=";X$(H4)
390    FOR J=1 TO Jbt(H4)
400      IF B1(H4,J) THEN
```

```
410       PRINT USING Picmpi;J;Nc$(B1(H4,J));B2(H4,J)
420     ELSE
430       PRINT USING Picmpi;J;"Digit=";B2(H4,J)
440     END IF
450     IF J MOD 3=0 THEN PRINT
460   NEXT J
470   PRINT
480   PRINTER IS Prn1
490   RETURN
500 Lacmp:La$=Cmp$(H4)
510   GOSUB Rcmp9
520   IF Z=0 THEN Z=Z0
530   La$=TRIM$(La$[Z+1])
540   RETURN
550 Rcmp9:La$=TRIM$(La$)
560   Z0=POS(La$,"=")
570   Z=POS(La$,";")
580   RETURN
590 Icmp0:La$=Cmp$(H4)!  From menu
600 Icmp2:ON ERROR GOTO Icmp131
610   GOSUB Rcmp9
620   Q0$=La$[Z0+1]
630   IF Z>1 THEN Q0$=La$[Z0+1,Z-1]
640 Icmp5:X1$=""
650   X$(H4)=""
660   Jb=0
670   Jbt(H4)=0
680   Ierr=0
690   GOSUB Icmp9
700   GOTO Ck00
710 Icmp9:K1=POS(Q0$," ")
720   IF K1=0 THEN RETURN
730   Q0$=Q0$[1,K1-1]&Q0$[K1+1]
740   GOTO Icmp9
750 Icmp10:GOSUB Scmp
760   IF J0<=Pcolmax THEN
770     R1=1
780     GOSUB Icmp17
790     GOSUB Ck12
800     RETURN
810   ELSE
820     Q1$=UPC$(Q$)!  For total iron.
830     IF Q1$="T.FE2O3" OR Q1$="T.FEO" THEN
840       Q$="Fe2O3"
850       GOSUB Scmp
860       IF J0<=Sc(4) THEN
870         J1=J0
880         Q$="FeO"
890         GOSUB Scmp
900         IF J0<=Sc(4) THEN
```

```
910           J2=J0
920           IF Q1$="T.FE2O3" THEN
930             R1=1
940             R2=1.11134
950             IF Chrat$="M" THEN R2=.5
960           END IF
970           IF Q1$="T.FEO" THEN
980             R1=.899811
990             IF Chrat$="M" THEN R1=2
1000            R2=1
1010          END IF
1020          J0=J1
1030          GOSUB Icmp17
1040          J0=J2
1050          R1=R2
1060          GOSUB Icmp17
1070          Q8$="(X+X)"
1080          Q9$=Q8$
1190          GOSUB Ck121
1100          RETURN
1110        END IF
1120      END IF
1130    END IF
1140 Icmp131:PRINT "*** ";Q$;" NOT FOUND"
1150    GOTO Ck19
1160  END IF
1170 Icmp17:IF Jbt(H4)<=Nterm THEN
1180    Jbt(H4)=Jbt(H4)+1
1190    B1(H4,Jbt(H4))=J0
1200    B2(H4,Jbt(H4))=R1
1210    RETURN
1220  ELSE
1230    PRINT "* TERMS OVER";Nterm
1240    GOTO Ck18
1250  END IF
1260 Scmp:FOR J0=1 TO Pcolmax!  Searching a component in the component-file.
1270    IF UPC$(Nc$(J0))=UPC$(Q$) THEN RETURN
1280  NEXT J0
1290  RETURN
1300 Ck00:K0=1
1310  Len=LEN(Q0$)
1320  IF Len=0 THEN Ck18
1330 Ck01:FOR K1=K0 TO Len
1340    Q1$=Q0$[K1;1]
1350    RESTORE Ckda1
1360    GOSUB Ck90
1370    IF Ope THEN
1380      IF K1=K0 THEN
1390        Q8$=Q0$[K1;1]
1400        Q9$=Q0$[K1;1]
```

```
1410          IF X1$="X" AND Q8$="(" OR X1$=")" AND Q8$="(" THEN Q8$="*"&Q8$
1420          GOSUB Ck13
1430          IF K1>=Len THEN Ck16
1440          K0=K1+1
1450          GOTO Ck01
1460        ELSE
1470          GOTO Ck103
1480        END IF
1490      END IF
1500    NEXT K1
1510  Ck103:Q1$=Q0$[K0,K1-1]
1520    Len2=LEN(Q1$)
1530    Ng=0
1540    Pg=0
1550    FOR K2=1 TO Len2!  Searching coefficient or constant.
1560      Q2$=Q1$[K2;1]
1570      IF Q2$>="0" AND Q2$<="9" OR Q2$="." THEN Ck2
1580      IF K2=1 THEN Ck5
1590      GOTO Ck4
1600  Ck2:Ng=Ng+1!  Digit found.
1610      IF Q2$="." THEN Pg=Pg+1
1620  Ck3:IF Pg>1 THEN Ck4
1630    NEXT K2
1640    IF Ng=1 AND Pg=1 THEN Ck5
1650  Ck4:R1=VAL(Q1$[1,K2-1])!  Separating coeffient from the component.
1660    GOSUB Ck11
1670    IF K2<=Len2 THEN
1680  Ck5:IF K2+1<=Len2 THEN !  Logarithm: log and ln.
1690        IF UPC$(Q1$[K2;2])="LN" THEN
1700          Q9$="N"!  Operation-code for ln is "N" and log "L"
1710          K2=K2+2
1720        END IF
1730        IF K2+2<=Len2 AND UPC$(Q1$[K2;3])="LOG" THEN
1740          Q9$="L"
1750          K2=K2+3
1760          Q8$=Q9$
1770          GOSUB Ck121
1780        END IF
1790      END IF
1800      IF K2<=Len2 THEN
1810        IF Q2$="[" THEN Ck14!  Characters wrapped by brackets are
absolutely defined as a component.
1820        Q$=Q1$[K2,Len2]
1830        Q1$=Q$
1840        GOSUB Icmp10
1850        IF Ierr THEN RETURN
1860      END IF
1870    END IF
1880  Ck6:IF K1<=Len THEN
1890      K0=K1
```

```
1900    GOTO Ck01
1910 Ck11:J0=0 !  Digit
1920    GOSUB Icmp17
1930 Ck12:Q8$="X" !  Encoding, or building an operation-code.
1940    Q9$="X"!  Inserting a multiplication symbol if omitted in the given
expression.
1950 Ck121:IF X1$=")" OR X1$="X" THEN Q8$="*"&Q8$
1960 Ck13:X$(H4)=X$(H4)&Q8$
1970    X1$=Q9$
1980    RETURN
1990 Ck14:K1=K0+K2
2000    Z=POS(Q0$[K1],"]")
2010    IF Z=0 THEN Ck18
2020    Q$=Q0$[K1,K1+Z-2]
2030    GOSUB Icmp10
2040    IF Ierr THEN RETURN
2050    IF K1+Z<=Len THEN
2060      K0=K1+Z
2070      GOTO Ck01
2080    END IF
2090  END IF
2100 Ck16:IF Ierr THEN RETURN!  Checking the operation-code.
2110  Len=LEN(X$(H4))
2120  Ierr=0
2130  Np=0
2140  Ng=0
2150  FOR K1=1 TO Len
2160    Q1$=X$(H4)[K1;1]
2170    IF K1=1 THEN
2180    ELSE
2190      IF X$(H4)[K1-1;1]="(" THEN
2200        RESTORE Ckda4
2210        GOSUB Ck90
2220        IF Ope THEN Ck18
2230      END IF
2240    END IF
2250    IF K1<Len THEN
2260      IF Q1$="^" AND X$(H4)[K1+1;1]<>"X" THEN Ck18
2270    END IF
2280    IF Q1$="(" THEN Np=Np+1
2290    IF Np>Npar THEN
2300      PRINT "* PARENTHESES OVER";Npar
2310      GOTO Ck18
2320    END IF
2330    IF Q1$=")" THEN Np=Np-1
2340    IF Np<0 THEN Ck17
2350    RESTORE Ckda3
2360    GOSUB Ck90
2370    IF Ope THEN Ng=Ng+1
2380    IF Ng>1 THEN Ck18
```

```
2390    IF Ope=0 THEN Ng=0
2400  NEXT K1
2410  Q1$=X$(H4)[Len]
2420  RESTORE Ckda2
2430  GOSUB Ck90
2440  IF Ope THEN Ck18
2450  IF Np=0 THEN Ck20!  Pass checking.
2460 Ck17:PRINT "*** MISSING ";CHR$(34);
2470  IF Np>0 THEN PRINT ")";
2480  IF Np<0 THEN PRINT "(";
2490  PRINT CHR$(34);" in ";Q0$
2500  GOTO Ck19
2510 Ck171:PRINT "** ERROR No.=";ERRN
2520 Ck18:PRINT "*** ";Q$;" NOT ALLOWED"
2530 Ck19:Ierr=1
2540  PRINT
2550  GOSUB Beep1
2560 Ck20:OFF ERROR
2570  RETURN
2580 Ckda1:DATA +,-,*,/,(,),^,@
2590 Ckda2:DATA L,N
2600 Ckda3:DATA +,-
2610 Ckda4:DATA *,/,^,@
2620 Ck90:Ope=0
2630  READ Z$
2640  IF Z$="@" THEN RETURN
2650  IF Z$=Q1$ THEN Ope=9
2660  GOTO 2630
```

2.2. Operations of Calculation along the Operation-Code.

Variables: P(*)--Numerical data of a sample. Plt(*)--Result of calculation. Q(*)--Numerals under calculation. Pa(*)--Informations for parentheses. Nd--No data (defined as 9.0E+63).

```
2670 Pk0: ! [PK16] = CALC  84X12
2680  ON ERROR GOTO Pk51
2690  Plt(H4)=Nd
2700  FOR Jb=1 TO Jbt(H4)!  Enter the component-number and values of
constant into Q(*) to prepare for calculations.
2710     IF B1(H4,Jb) THEN
2720        IF P(1,B1(H4,Jb))>=Nd THEN Pk52
2730        Q(Jb)=B2(H4,Jb)*P(1,B1(H4,Jb))
2740     ELSE
2750        Q(Jb)=B2(H4,Jb)
2760     END IF
2770  NEXT Jb
2780 Pk03:Ope=0
```

```
2790  Jp=0
2800  Ierr=0
2810  Jb=0
2820  Jc=0
2830  Fnc=0
2840  Len=LEN(X$(H4))
2850  FOR K1=1 TO Len
2860    Q1$=X$(H4)[K1;1]
2870    IF Q1$="+" THEN Ope=1
2880    IF Q1$="-" THEN Ope=-1
2890    IF Q1$="*" THEN Ope=2
2900    IF Q1$="/" THEN Ope=-2
2910    IF Q1$="L" THEN Fnc=1
2920    IF Q1$="N" THEN Fnc=2
2930    IF Q1$="X" THEN
2940      Jb=Jb+1
2950      Jc=Jc+1
2960      J1=Jb
2970      GOSUB Pk2
2980    END IF
2990    IF Q1$="(" THEN!  Enter the informations into the parantheses array.
3000      Jp=Jp+1
3010      Pa(1,Jp)=Jc+1
3020      Pa(2,Jp)=Ope
3030      Pa(3,Jp)=Fnc
3040      Ope=0
3050      Fnc=0
3060    END IF
3070    IF Q1$=")" THEN!  Totalizing the values wrapped parentheses and
calculation is held according to values of Ope and Fnc.
3080      J1=Pa(1,Jp)
3090      GOSUB Pk6
3100      Q(J1)=Z
3110      Jc=J1
3120      Ope=Pa(2,Jp)
3130      Fnc=Pa(3,Jp)
3140      GOSUB Pk2
3150      Jp=Jp-1
3160    END IF
3170    IF Ierr THEN Pk52
3180  NEXT K1
3190  J1=1
3200  GOSUB Pk6
3210  Plt(H4)=Z
3220  GOTO Pk52!.CALC END
3230 Pk2:IF K1<Len THEN
3240    IF X$(H4)[K1+1;1]="^" THEN
3250      Jb=Jb+1
3260       Q(J1)=Q(J1)^Q(Jb)
3270      K1=K1+2
```

```
3280    END IF
3290  END IF
3300  IF Fnc THEN
3310    IF Q(J1)<=0 THEN Pk51
3320    ON Fnc GOSUB Pk70,Pk71
3330    Fnc=0
3340  END IF
3350  ON ABS(Ope)+1 GOTO Pk23,Pk3,Pk4
3360 Pk23:Q(Jc)=Q(J1)
3370  RETURN
3380 Pk3:Q(Jc)=Q(J1)*Ope
3390  RETURN
3400 Pk4:Jc=Jc-1
3410  IF Ope=-2 THEN
3420    IF Q(J1)=0 THEN Pk51
3430    Q(J1)=1/Q(J1)
3440  END IF
3450  Q(Jc)=Q(Jc)*Q(J1)
3460  RETURN
3470 Pk6:Z=0
3480  FOR J0=J1 TO Jc
3490    Z=Z+Q(J0)
3500  NEXT J0
3510  RETURN
3520 Pk70:Q(J1)=LGT(Q(J1))!  Logarithmic functions.
3530  RETURN
3540 Pk71:Q(J1)=LOG(Q(J1))
3550  RETURN
3560 Pk51:Ierr=1
3570 Pk52:OFF ERROR
3580  RETURN
3590 Joint: END
```