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VOLCANIC METALLOGENIC DATABASE

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ABSTRACT

Work has begun on a computer database that will hold all available, good-quality, public-domain geochemical data on volcanic rocks for Newfoundland and Labrador. The structure of the database has been completed and data inputting/importing has begun. The data will be held in two main tables; the FIELDDAT table will store descriptive data for each sample such as rock type, location and unit; the GEOCHEM table will hold the analytical results, and related information such as the method of analysis, year of analysis and analytical laboratory. Ancillary tables will hold additional information such as explanations of abbreviations. The tables can be combined so that data from both the main tables can be viewed together. A user will be able to select data by sample number, rock type, unit, NTS, geologist, element or oxide, method of analysis, priority, year of analysis or analytical laboratory or any combination of these factors. Forms for manual input of data and reports for output of data to file or printer have been designed.

INTRODUCTION

During the past year, work began on a geochemical database for volcanic rocks in Newfoundland and Labrador. The structure of the database has recently been completed and the input of data has begun. This paper describes, in general terms, the database structure and methods of inputting/importing and outputting/exporting data.

PROJECT SCOPE AND OBJECTIVES

The aim of the project is compilation of all available good-quality, public-domain geochemical data on volcanic rocks for both insular Newfoundland and Labrador. This will include provincial- and federal-survey data, and data from theses. Analyses from assessment reports may be included if they are found to be of good quality and contain sufficient controls.

Where an element has been analyzed by more than one method, results for each method will be included and data will be ranked according to reliability of the particular method for each element.

The database will provide a repository for a broad spectrum of geochemical data and is particulary aimed at users for whom the geochemistry of volcanic rocks is a useful mineral-exploration tool, i.e., those engaged in the search for base-metal, massive-sulphide deposits.

DATABASE STRUCTURE

The database software is R-base 3.1, a relational database system designed to run on an MS-DOS microcomputer. The data are contained in a series of tables, which can be linked in a variety of ways. Two main tables (Table 1) hold the data—one contains descriptive data for the samples, such as location, rock-type or owner, and the other contains the analytical data. Ancillary tables (e.g., Table 2) contain helpful information, such as preferred listing order of elements and explanations of abbreviations. The tables can be linked so that the user can see data from more than one table at the same time.

Data can be imported from an ASCII file or spreadsheet or can be input manually via a form or directly into the table. It can be exported directly to a file or can be formatted in a report for export to a file or printer.

MAIN TABLES

Table 1 (FIELDDAT) contains descriptive data in the following columns:

COLUMN	TYPE	WIDTH	
Labnum	*integer*	7	
Fieldnum	*text*	8	
Unit	*text*	*	group or complex
Subunit	*text*	*	formation or member
NTS	*text*	5	
UTMeast	*integer*	6	
UTMnorth	*integer*	7	
Zone	*integer*	2	
Rocktype	*text*	4	four-letter code
Owner	*text*	*	project geologist
Age	*text*	*	
Altered	*integer*	1	code for alteration level
Restrict	*text*	1	Y or N to restrict access
Info	*note*	*	comments—e.g., DDH numbers

* indicates that the column width will be expanded as necessary to accommodate text as full names are used rather than codes.

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Table 1. Main tables—FIELDDAT contains descriptive data for each sample and GEOCHEM contains the analytial data. Some typical data are shown. Refer to Table 2 for explanations of abbreviations and to text for discussion of columns; -0- indicates a null value.

FIELDDAT

Labnum	Fieldnum	Unit	Subunit	NTS	Zone	Utmeast	Utmnorth
1543292	BK87014	Lushs Bight Group	Pillow lava member	2E12	21	576220	5494540
1543006	DE85045	Victoria Lake Group	-0-	12A16	21	576950	5407000
1543002	DE85007						

Rocktype	Owner	Age	Restrict	Altered	Info
etc.					
BSLT	B.Kean	Ordovician	n	3	Little Bay glory hole
BSLT	D.Evans	Ordovician	n	1	-0-
BSLT	D.Evans	Ordovician	n	1	-0-

GEOCHEM

Labnum	Fieldnum	Element	Method	Result	Priority	Labcode	Year	Allmeth
1543292	BK87014	SiO_2	AAS	48.25	1	NDM	1987	AAS
1543292	BK87014	TiO_2	AAS	0.70	1	NDM	1987	AAS
1543292	BK87014	La	ICM	0.93	1	MUN	1989	ICM, ICS
1543292	BK87014	La	ICS	1	2	NDM	1988	ICM, ICS
etc.								

For ease of use, columns such as *Unit, Subunit* and *Age* will contain full names rather than abbreviations or codes. The *Rocktype* column contains a four-letter code in order to ensure compatibility with other in-house databases.

Table 1 (GEOCHEM) contains the analytical data in the following columns:

COLUMN	TYPE	WIDTH	
Labnum	*integer*	7	
Fieldnum	*text*	8	
Element	*text*	5	
Method	*text*	3	code for analytical method
Result	*double*	*	variable no. of decimal places
Priority	*integer*	1	rank of analytical method
Labcode	*text*	3	code for analytical laboratory
Year	*integer*	4	year of analysis
Allmeth	*text*	*	list of methods for element

All analyses in Table 1 (GEOCHEM) are contained in one column—*Result*, and the element or oxide is identified by the column *Element*. The column *Priority* provides the user with a quick method of selecting the best data for each sample. This is achieved by assigning a value of 1 to the best method of analysis of an element for a particular sample. For example, Zr by X-ray fluoresence (XRF) might be ranked 1 and Zr by inductively-coupled plasma spectrometry (ICS) ranked 2 for a particular sample; another sample might have been analyzed for Zr by ICS (ranked 1) and by atomic absorption spectrometry (AAS) (ranked 2). Niobium by ICS might be ranked 1 and Nb by AAS, ranked 2. The column *Allmeth* lets the user see at a glance whether an element has been analyzed by more than one method. The user could, therefore, select all priority 1 data or select all data resulting from a particular method.

Because the elements and oxides are listed as values in a column rather than as column headers, each sample number in the GEOCHEM table is repeated as many times as there are individual analyses for that sample (Table 1). In the FIELDDAT table, each sample number exists only once. The FIELDDAT:GEOCHEM tables, therefore, have a one-to-many relationship.

ANCILLARY TABLES

Helpful information is contained in several small subordinate tables (e.g., Table 2). The most important table is called CLASSIFY. This table holds information about elements and oxides and provides a means of contro.ling the selection and display of geochemical data. It contains the following columns:

Table 2. Ancillary tables that contain helpful information. Abbreviations in *Subcateg* and *Category* columns: TE–transition element, MET–metallic element, LFS–low field strength element, OXI–oxide, MAJ–major element, TRA–trace element. Other abbreviations as shown

CLASSIFY

Element	Atomic#	Weight	Subcateg	Sequence	Printout	Category
Si	14	28.086	-0-	-0-	n	MAJ
Cr	24	51.996	TE	18	y	TRA
Zn	30	65.37	MET	25	y	TRA
Rb	37	85.47	LFS	47	y	TRA
SiO_2	-0-	60.07	OXI	1	y	OXI
etc.						

ROCK

Rocktype	Rockname
ANDS	andesite
BSLT	basalt
DACT	dacite
DIAB	diabase
FLST	felsite
etc.	

ANALYST

Labcode	Labname
BCQ	Becquerel
CHX	Chemex
NDM	Nfld. Dept Mines & Energy
GSC	Geol. Survey of Canada
MUN	Memorial Univ. of Nfld.
etc.	

METHOD

Method	Analmeth
AAS	Atomic Absorption Spectrometry
ICM	Inductively Coupled Plasma-Mass Spectrometry
ICS	Inductively Coupled Plasma Emmission Spectrometry
INA	Instrumental Neutron Activation Analysis
XRF	X-ray Fluorescence
etc.	

COLUMN	TYPE	WIDTH	
Element	*text*	5	
Atomic#	*text*	3	
Weight	*double*	*	atomic or molecular weight
Subcateg	*text*	3	HFS or REE etc.
Sequence	*integer*	2	listing order (SiO_2 = 1)
Printout	*text*	1	Y or N to select element
Category	*text*	3	OXI, MAJ or TRA

Column *Category* lets a user distinguish between major and trace elements; *Subcateg* further subdivides the trace elements, e.g., high-field strength (HFS) or rare-earth elements (REE). Column *Printout* can be used to select or reject each element for output to a file or printer. Column *Sequence* controls the order in which elements are listed in certain reports and applications.

Tables METHOD, ROCK, and ANALYST provide explanations of abbreviations used in the two main tables and ensure consistent use of these codes. Table ROCK for example would contain only 2 columns:

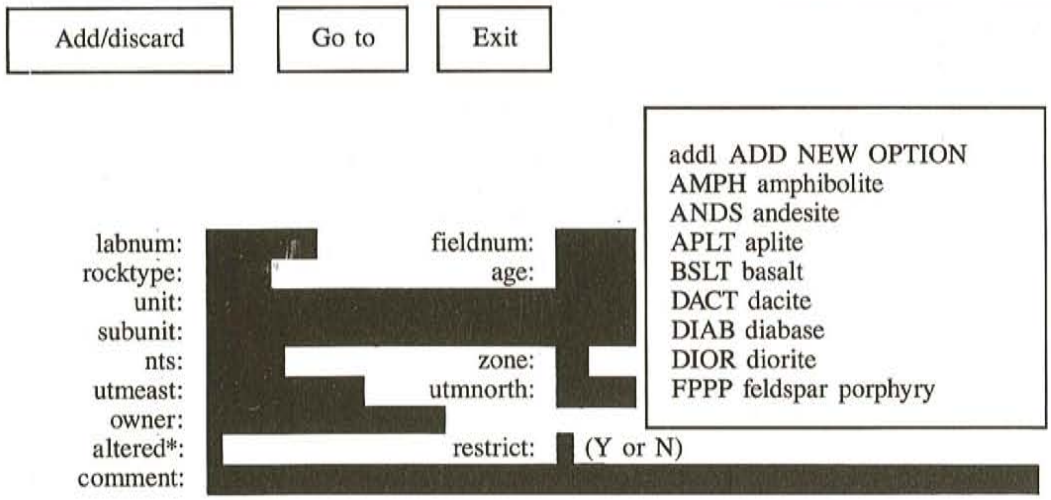
COLUMN	TYPE	WIDTH	
Rocktype	*text*	4	code e.g. BSLT
Rockname	*text*	*	full name e.g. basalt

Tables METHOD and ANALYST similarly contain 2 columns of abbreviations and full names (Table 2).

SELECTING DATA

The two main tables, along with the CLASSIFY table, can be combined into a view that lets the user access all data. A user will be able to select data by sample number, rock type, unit, NTS, element or oxide, method of analysis, priority, year of analysis or analytical laboratory or any combination of these factors. The elements/oxides can be selected on an individual basis or by using the *Category* or *Subcateg* columns of the CLASSIFY table. A user can quickly select all data for a particular sample or can select only priority 1 data or only data that have been analyzed by a particular method. The results of the selection can then be saved into another table or output to another file or to the printer.

Table 3. Form FLDFORM, which is used to input data into the FIELDDAT table. Each field represents a column in the table. (The comment field loads the *Info* column). Shown at right is a pop-up menu that provides the user with the correct abbreviation for each rock type. The selected four-letter code is automatically loaded into the *Rocktype* field. The user can add a new code if needed



For pop-up menu highlight option (use arrow, mouse or 1st letter) and press [enter]. Press [esc] to abort.

* for altered field enter:
0–fresh
1–normal greenschist alteration
2–excessively altered
3–alteration related to mineralization
[enter]–unknown (leaves field null)

IMPORTING DATA

Data can be imported into the database from an ASCII file or from a spreadsheet. Because the structure of the GEOCHEM table differs significantly from standard geological format, data for this table must first be transposed into the correct format. This is most easily accomplished via a spreadsheet. Most Department of Mines and Energy data are already available in SPSS format, which can easily be imported into Lotus 123. Data can then be cleaned up and put into the proper format using a macro. Information such as method of analysis or year of analysis can be entered at this stage or can be entered later into R-Base. The best approach to this depends, to some extent, on the characteristics of each dataset. Some department data exist as separate files divided on the basis of analytical laboratory or year of analysis. Other datasets contain all data for an area regardless of how, when or where the samples were analyzed. The user may have to spend considerable time trying to sort out such details or trying to track down missing data such as UTM coordinates. The cooperation of the project geologist is of great importance at this stage.

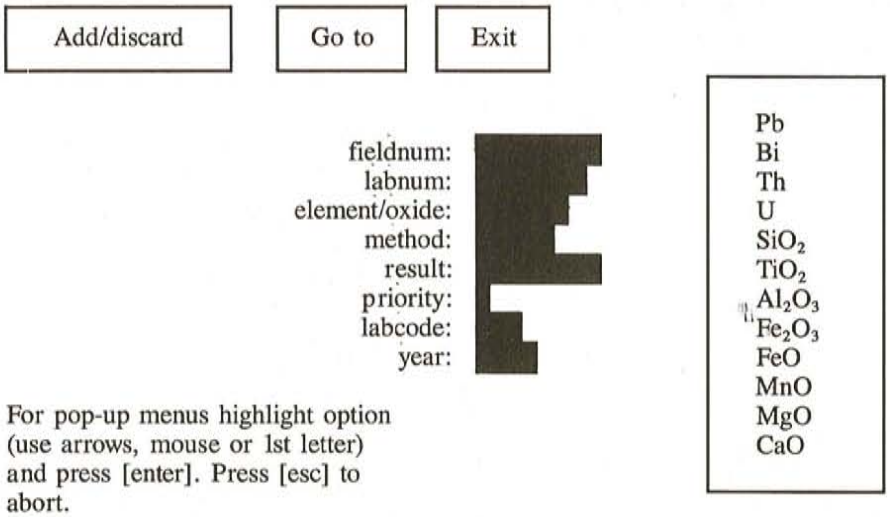
Data can also be exported from R-base into other packages or into ASCII format, however, it is generally necessary to first select the desired information and put it into standard geological format using a report (see Reports section further on).

FORMS

Standardized forms for manual input of data have been designed and will be used where data are not available in electronic format. A form called FLDFORM loads data into the FIELDDAT table. The *Rocktype* field has an automatic pop-up menu that provides the user with the proper abbreviation for each rock type (Table 3). The user can add a new option to this pop-up menu if the desired rock type is not already listed.

Another form called CHEMFORM (Table 4) loads analytical data into the GEOCHEM table. To speed up the input of data, the form can be set up so that certain fields contain default values, e.g., if all analyses to be typed in were acquired in 1988, the Year field could be set to this value. A field can also be set to duplicate the value in the previous row so, for example, the sample numbers would only have to be typed in once for each sample. A pop-up menu in the CHEMFORM form (Table 3) lists elements and oxides to speed their input into the *Element* field in the GEOCHEM table. Only the elements of interest are displayed. This is accomplished by use of a form called PRINFORM that loads the *Printout* column in the CLASSIFY table with either 'y' to include an element or 'n' to exclude it. This can also be used to select elements for inclusion in views and reports.

Table 4. Form CHEMFORM, which is used to input data into the GEOCHEM table. The pop-up menu at right speeds up the entry of element/oxide names



REPORTS

Two basic types of reports have been designed. The first, called LISTREP, produces a one-sample per-page report (Table 5) that contains all selected geochemical data from the GEOCHEM table, as well as descriptive data from the FIELDDAT table, such as rock type, unit and location. The driving view for this report is called PRINVIEW and combines the tables GEOCHEM, FIELDDAT, and CLASSIFY. Data can be restricted by any column, e.g., *Unit, NTS, Rocktype, Priority,* etc., by building this view to contain only the desired data or by using quick select from the report printing menu. Elements can be selected on an individual basis by using the form PRINFORM or on a group basis by using the columns *Category* or *Subcateg.* The data would ideally be sorted from the report printing menu, e.g., by *Unit, Subunit, Rocktype, Labnum* and *Sequence.* Sorting by *Sequence* is necessary if the user wishes to have the components listed in standard order (SiO_2, TiO_2, Al_2O_3, etc.). Sorting by *Element* would not work as this would result in an alphabetical listing (Ag, Al_2O_3, As, etc.). This report presents both hydrous and anhydrous data and lists the method and year of analysis and the analytical laboratory. The column *Allmeth* is also listed to let the user see if any additional data exist for a particular element.

The second type of report called ARRAYREP produces a listing in standard geological format (Table 6) for export to programs such as IGPET. For this report, data must be transformed by use of variables (lookups) to achieve the desired format; as a result, if the number of elements is greater than about 23, more than one report must be used to avoid memory problems. In practice it would be most convenient to put all major elements in one report and all trace elements in another report. If the data are to be printed, the number of elements per report will be limited by the width of the paper. If the data are to be exported to IGPET, the user must first decide what method of analysis (normally priority 1) to select for each element as IGPET can only hold one analysis per sample for each element. The driving table for this report is the FIELDDAT table; this table is required because it contains only one occurrence of each sample number in the Labnum column. Data can be limited by, or sorted by, columns within this table at the report printing menu. However, in order to limit data by method, laboratory, priority etc., a temporary table called PRINTTAB must be built. This table will hold a subset of the GEOCHEM table and will significantly reduce processing time. The lookup variables that hold the data are expressions such as:

SiO_2=result in Printtab where labnum=labnum and element=SiO_2

Each column in the resulting report is the product of such an expression.

DISCUSSION

This database has been designed to be flexible and easy to use. The most difficult problem has been how to provide the user with all pertinent information that is necessary to evaluate the quality and comparability of analyses. This includes such parameters as method of analysis, year of analysis and analytical laboratory. An additional complicating factor is the analysis of some samples for a particular element by more than one method. The need to accommodate these factors was the reason for the unconventional format of the GEOCHEM table. This format has two main disadvantages:

- importing/exporting to and from other packages is more complex because existing electronic data are generally in standard geological format or are required to be for input to packages such as IGPET; and

- the number of rows in the GEOCHEM table is greatly increased; this combined with the duplication

Table 5. Sample output from LISTREP report, which provides a one-sample-per-page printout. Both raw and recalculated (anhydrous) data are shown. In this example, AAS and ICS analyses were selected. The *Allmeth* column lets the user know that several elements have also been analyzed by XRF. See Table 2 for codes

Fieldnum: SS015
Labnum: 1341051
Rocktype: trondhjemite
NTS: 12H10

Unit: Gull Lake intrusive suite
Subunit: Black Duck Ponds trondhjemite
Geologist: W.R. Smyth
UTMeast: 506200 UTMnorth: 5498750

Component	Result	Recalc	Meth	Lab	Year	AllMeth*
SiO_2	74.8	75.41	AAS	NDM	1981	AAS
TiO_2	0.31	0.31	AAS	NDM	1981	AAS
Al_2O_3	12.8	12.90	AAS	NDM	1981	AAS
Fe_2O_3	1.29	1.30	AAS	NDM	1981	AAS
FeO	1.84	1.85	AAS	NDM	1981	AAS
MnO	0.06	0.06	AAS	NDM	1981	AAS
MgO	0.72	0.72	AAS	NDM	1981	AAS
CaO	1.16	1.16	AAS	NDM	1981	AAS
Na_2O	5.4	5.44	AAS	NDM	1981	AAS
K_2O	0.76	0.76	AAS	NDM	1981	AAS
P_2O_5	0.05	0.05	AAS	NDM	1981	AAS
LOI	1.41	1.42		NDM	1981	
Total	100.6	101.42		NDM		
Cu	1.	1.00	AAS	NDM	1982	AAS
Pb	1.	1.00	AAS	NDM	1982	AAS
Zn	27.	27.22	AAS	NDM	1982	AAS
Ag	1.	1.00	AAS	NDM	1982	AAS
Rb	12.	12.09	AAS	NDM	1982	AAS, XRF
Ba	55.	55.44	AAS	NDM	1982	AAS, ICS, XRF
Ba	79.	79.64	ICS	NDM	1988	AAS, ICS, XRF
Sr	68.	68.55	AAS	NDM	1982	ICS, XRF, AAS
Sr	80.	80.65	ICS	NDM	1988	ICS, XRF, AAS
Li	24.	24.19	AAS	NDM	1982	AAS
Nb	4.	4.03	ICS	NDM	1988	ICS, XRF
Zr	71.	71.57	ICS	NDM	1988	XRF, ICS
Y	13.	13.10	ICS	NDM	1988	ICS, XRF
Th	0.	0.00	ICS	NDM	1988	ICS, XRF

* Analytical methods in *Allmeth* column listed in order of priority.

of sample numbers in the key *Labnum* column slows down searches and sorts.

However, there are many advantages to the format:

- all pertinent information is included;
- the number of columns is significantly reduced; an alternative structure (separate columns for each method of analysis of each element) would result in an unwieldy number of columns;
- the amount of wasted (null) space is greatly reduced; the alternative structure described above would be inefficient in that if only 50 samples out of several thousand had been analyzed for Co by atomic absorption most of the Co-AAS column would contain nulls;
- data may be selected or sorted by any number of parameters such as NTS, unit, rock type, method of analysis, etc;
- it is easy to determine, without any prior knowledge, what type of data exist for any particular sample, or for any particular area or rock unit; and
- this structure is easily adapted for use with other types of data, e.g. soil geochemistry.

Table 6. Sample output from ARRAYREP report, which lists data in standard geological format. Priority 1 data have been selected. Generally, major elements would be included in one report and trace elements in another report as there is a limit of about 23 elements due to memory limitations. The dashed line indicates a null value. The user can choose the method of displaying nulls

'Sample'	'SiO_2'	'TiO_2'	'Al_2O_3'	'Fe_2O_3'	'LOI'	'Cr'	'Cu'	'Zn'	'Ba'	'Rb'
1543001	61.20	0.95	14.87	1.25	3.84	9	702	128	28	9
1543002	52.90	0.59	14.77	0.82	7.71	199	59	130	189	7
1543004	83.45	0.13	8.40	----	0.51	4	27	17	338	22
1543009	47.40	2.06	16.78	1.34	3.36	134	68	76	51	7
1543011	46.90	2.00	16.17	1.58	2.94	174	68	90	58	8
1543012	45.60	2.06	15.53	2.11	3.47	176	75	90	42	11
1543013	46.70	2.25	16.88	2.38	2.65	53	62	90	54	15
1543014	47.40	1.73	15.95	1.33	2.87	215	71	76	48	13

FUTURE CONSIDERATIONS

Although the structure is essentially complete, there are other problems yet to be solved such as the method of handling controls (standards and duplicates) and the establishment of a methodology for evaluating, assessing and reporting relative data quality. This will be more easily accomplished after a considerable amount of data has been loaded into the database. Other parameters may be further modified or refined. For example, the method of analysis as currently coded gives no indication of the type of sample dissolution that was used. This could be indicated by further refinement of the codes used or by addition of another column to hold such information. The GEOCHEM table may eventually have to be subdivided into smaller tables based on geographic regions, such as 1:250 000 or 1:50 000 map sheets because of the large number of rows. Longer term considerations include design of applications to make querying or adding data easier for those not familiar with R-base. These problems will require consultation with other members of the Department and other industry, government and university personnel—questions, comments and helpful hints are welcomed.

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