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INFOREX-3.0: A DATABASE ON EXPERIMENTAL STUDIES OF PHASE EQUILIBRIA IN IGNEOUS ROCKS AND SYNTHETIC SYSTEMS: I. DATAFILE AND MANAGEMENT SYSTEM STRUCTURE

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Abstract—INFOREX-3.0 is a sophisticated database manager for igneous petrologists and geochemists. It is designed as an aid in searching the published experimental database, and extracting specific subsets of that data. In addition, the program allows the user to derive numerical mineral-melt expressions based on any dataset. Its major function is as a computerized melting-experiment reference manual that presents data in a fixed format, with key word search functions and flags as an integral part of the program. At present, the system accesses information on 162 experimental studies carried out from 1962 to 1994. The database includes 6174 individual runs with more than 8300 coexisting phase compositions for 30 minerals plus melt. Most of the data are "dry", but about 2200 include volatile components, such as H_2O and CO_2. INFOREX is hot-key driven, allowing users to sort easily and quickly through the data using any set of experimental conditions or rock type parameters. The main options include: (1) configuration of INFOREX; (2) extraction of general information on the current state of the system; (3) updating and editing the database files; (4) selection of run conditions of interest (setting rock types plus a range of pressures, temperatures, oxygen fugacities, run duration as well as types of containers and resultant phase assemblages); (5) setting phase assemblages (e.g., olivine-melt or garnet-spinel) for the selected set of experiments; (6) export/import operations; and (7) calculation of mineral-melt geothermometers. The INFOREX database is a powerful tool for the use in the development of petrogenetic models by providing the ability to manipulate easily accessed mineral-melt equilibria data.

Key Words: Experimental data, Phase equilibria, Database, Management system.

INTRODUCTION

The experimental investigation of phase equilibria in natural and synthetic silicate systems is one of the basic fields of igneous petrology. Almost all petrologic models used for interpretation of the diversity of natural volcanic or intrusion rocks use experimental phase equilibria information. The development of microprobe analysis and advanced experimental techniques has produced literally thousands of major and trace element analyses of experimental runs. These data have been presented in the literature and are preserved in personal or institution databases around the world. This information, obtained at considerable expense, is a scientific resource of great importance for the further development of igneous petrology, especially in the field of geothermometry and computer simulation of magmatic differentiation processes (Nielsen, 1985, 1990; Ghiorso and Carmichael, 1985; Ariskin, Barmina, and Frenkel, 1987; Weaver and Langmuir, 1990; Ariskin and others, 1993; Ghiorso, Hirshmann, and Sack, 1994). At present, to use the available experimental data one has to navigate laboriously through the literature and evaluate the quality of the information case by case. This is regardless of the type of application. In fact the ability to test two-phase geothermometers and geobarometers available in the literature, or to develop them independently may require different criteria on data selection. There is a need therefore, for a quick and easy means to access and manipulate the experimental data, for a variety of applications such as, data selection by petrochemical criteria (igneous rock types), or by run conditions (temperature, pressure, or oxygen fugacity).

Our approach to this problem has been to develop an experimental database, and to make that database available to all interested investigators (Ariskin and others, 1992). The purpose of this paper is to present the INFOREX-3.0 database with an emphasis on the description of its architecture and data management system. Another goal is

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to provide more information to INFOREX users concerning the structure of the datafiles and on the details of the user interface (UI). A more detailed description of the experimental data available in INFOREX-3.0 (as many as 6200 experiments including more than 8300 coexisting phase compositions) is given in a companion paper, along with several examples of how the database can be used in modeling (Ariskin and others, 1996).

ORGANIZATION OF THE INFOREX DATABASE FILES

Although a primary goal of the development of INFOREX was to construct mineral-melt geothermometers for the models simulating magmatic differentiation processes (Ariskin, Barmina, and Frenkel, 1987; Ariskin and others, 1993), we developed the database so as to be useful for the full range of experimental studies in igneous petrology. Towards that end, the database was designed to have a structured, rather than flat-file, architecture. This is true for both the structure of the datafiles (Fig. 1) and the general organization of the INFOREX data management system (Fig. 2). In general, the INFOREX database files can be divided into three categories: basic datafiles, data management system files, and auxiliary files. The basic datafiles contain information on the reference source (BIBL.TXT file), experimental conditions and phase assemblages (CONDIT.EXP), phase compositions (LIQ.EXP, PLAG.EXP, SPIN.EXP, etc.), volatile components (VOLAT.EXP) and others. Examples of these files are given in Appendix 1. The data management system files are designed to store information on topics that users can access using the help functions, plus the general parameters of the INFOREX environment and configuration. These include working subsets of the names of phase composition files, rock types, and container materials. The auxiliary files facilitate the manipulation and data swapping among the basic datafiles using the UI. Usually, all but one of the auxiliary files are deleted after each working session. The only exception is the PROCESS.DAT file that is created for further thermodynamic processing of the mineral-melt or two mineral equilibria experimental data (see next section).

Structure and linkage of basic datafiles

All INFOREX database files contain ASCII alphanumeric records with fixed length. The basic unit or entity upon which the database is built is an

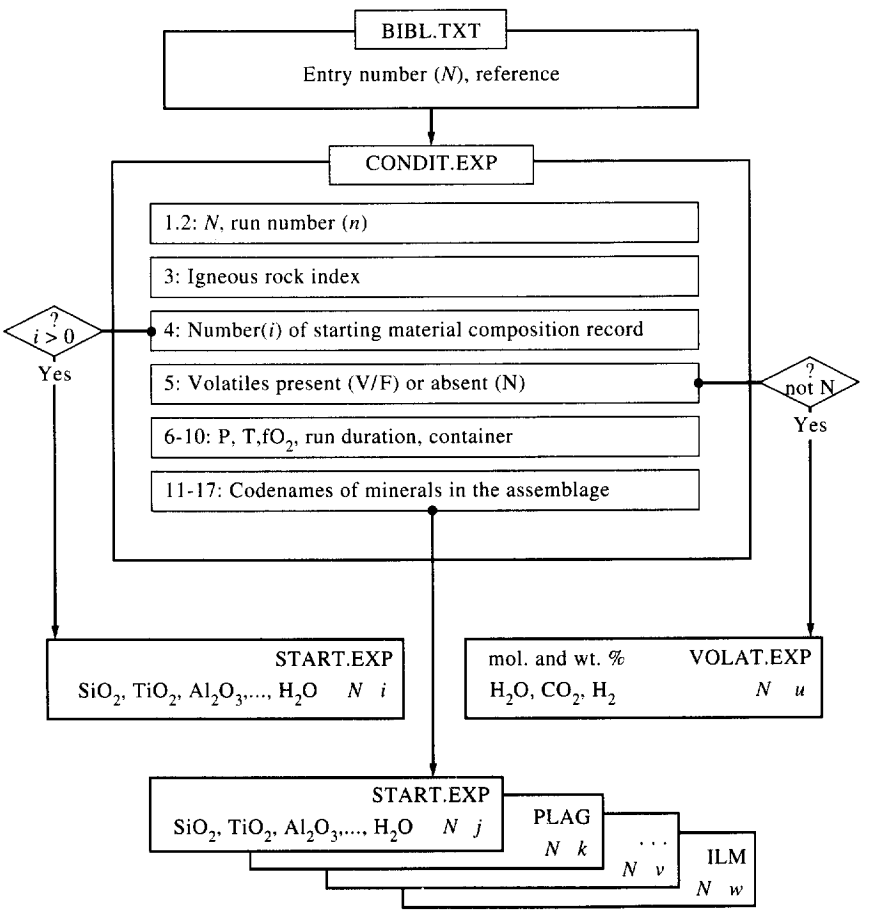

Figure 1. Structure of INFOREX database files. Letters *j, k, u, v, w* denote different run numbers.

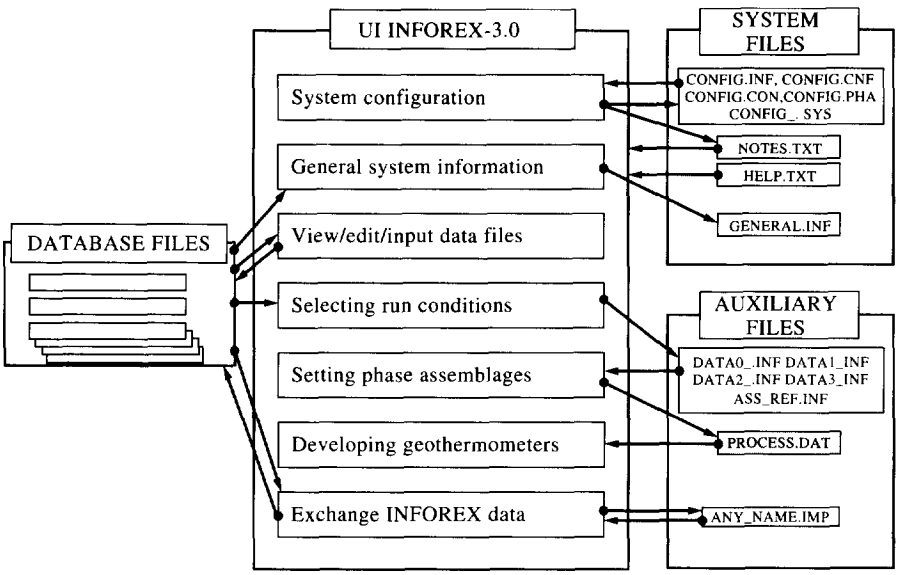

Figure 2. Structure of INFOREX-3.0 data management system.

individual experimental study. Each study has a reference record in the BIBL.TXT file and a set of master records in the CONDIT.EXP file (see Figure 1). Records in BIBL.EXP consist of up to four strings and include a working number and reference description (author, source, year, etc.). Note that the user can utilize any sequence of the bibliographic information if necessary. The same working number is given in the first column of the master records in CONDIT.EXP. This is used to link the master records to the BIBL.TXT file records. The second column in the CONDIT.EXP file represents the run numbers of the experimental study considered. Usually this run number corresponds to the sequence of run conditions and phase assemblages given in the literature tables in the source, but this sequence has been changed in instances where retention of the original numbers would have caused difficulty in the manipulation of the data.

The CONDIT.EXP master file records include essential information about each run, such as: (1) the type of igneous rock or synthetic system end members, (2) a reference number for the starting material which is linked to a composition in the START.EXP file, as well as (3) flag of the presence (*V*/*F*) or absence (*N*) of volatile components (where *F* denotes water saturated experiments and *V*—only undersaturated runs). These switches refer the user to the VOLAT.EXP file. Other important information fields are total pressure, temperature, oxygen fugacity, run duration, and up to seven codenames for the observed phases in the run products. In addition, the master record can include flags for special "water solubility" experiments (*WS*), where a value of water content in melt is available, or for estimated quantities of Fe^{3+} and Fe^{2+} species in the silicate glasses (*RE*). A number of other records are contained in additional subfiles linked to the main master record files.

The individual subrecords contain information on the experimental product compositions written in the form of regular and irregular formatted strings. Names of the "normally" formatted files are the abbreviations of mineral names with ".EXP" extensions (see Appendix 2). These files contain records formatted as twelve floating point number fields plus two integer number fields, which correspond to the basic experimental study and the current run number in BIBL.TXT and CONDIT.EXP files. The first twelve fields are to store contents of major oxides (in weight percents) in the sequence: SiO_2, TiO_2, Al_2O_3, FeO, MnO, MgO, CaO, Na_2O, K_2O, P_2O_5, Cr_2O_3, and H_2O (same format and sequence as in the START.EXP file). If the chemical composition of a phase is available, the flag in the main master record is set at "1" instead of as a space as the third character in the codename of a specific particular phase present in the assemblage. The irregularly formatted files were developed to store information that is beyond the scope of the normally formatted files. One of the most important files is VOLAT.EXP (see Figure 1). Subrecords of this file include weight and molar percents of H_2O, CO_2, and H_2 referenced to the bulk system (silicates + volatiles) or bulk volatile composition as well as the volatile component contents in a vapor phase (if present). The second irregular file shown in Figure 1 is MNLS.EXP. It was designed to accumulate phase compositions recalculated by authors to end-member component contents, such as forsterite for olivine, anorthite for plagioclase, etc. Our preference in creating this database was to store data that were as complete as possible.

Therefore, presentation of mineral compositions as endmembers only results in significant loss of information. Nevertheless, we have created these files so that even this rudimentary experimental information will not be lost, if other data on phase compositions are absent. The MNLS.EXP file is linked to the master record by the symbol "2" just after the indicator of a particular mineral phase. Two more irregular files are SULF.EXP and REDOX.EXP. The first one contains weight percent S, Fe, Mn, Ni, and Co—the major components of sulfide phases. The second file contains the estimated quantities of Fe^{3+} and Fe^{2+} species in the silicate glasses. They are linked to the main master record in CONDIT.EXP by using the codenames *SF* and *RE* respectively.

Data management system files

The core of INFOREX is composed of three types of system files: (1) files containing information on the INFOREX environment (general directory structure), (2) on-line help (HELP.TXT), and (3) a file termed NOTES.TXT that clears the main INFOREX abbreviations. The main environment file CONFIG.INF is located in the INFOREX root directory and consists of the records describing the current operating session...\DATA subdirectory. In the...\DATA subdirectory we have placed the second system file CONFIG.CNF, which contains four strings linked to four INFOREX directories developed to work with the individual system options (see below). These working directory pointers provide the user with the flexibility necessary to work simultaneously with different subsets of experimental data, for example with "volatile", "alkali basalt" or "high pressure" systems. The third group of data management system files were developed to store current working sets of igneous rock names (CONFIG.SYS), mineral phases (CONFIG.PHA) and container materials (CONFIG.CON). Note that the number of names given above is not limited, whereas the current configuration given in the NOTES.TXT file supports exactly fourteen different containers, 36 mineral phases, and 42 rock types. Thus, by using this specific configuration program option (see *SC*-option below) one can automatically customize the INFOREX system to work with any dataset.

DIRECTORY STRUCTURE AND DESCRIPTION OF USER INTERFACE

In this section, we describe the directory structure as set up by the normal installation procedure. The root INFOREX directory is initially named "D:\INFOREX\", where "D" represents a disk drive. It contains a set of executable files to be run by the main management program termed INFOMAN.EXE as well as some management system files. Basic experimental datafiles, BIBL.TXT file and configuration files are located in the "D:\INFOREX\DATA\" subdirectory. Two other subdirectories termed "D:\INFOREX\EXCHANGE\" and "D:\INFOREX\SAVE\" begin as empty ones after installation. The first one is created for *IMPORT/EXPORT* operations, to provide an easy exchange of experimental datafiles between different users. The second subdirectory serves to store general system information on the current state of the database—the GENERAL.INF file, as well as PROCESS.DAT file created for further thermodynamic calculations. Users can change the names of these subdirectories, but must keep its general structure intact. All changes are to be put into system files as will be discussed later.

The development of the INFOREX database started after the first models simulating magmatic differentiation processes were constructed (Ariskin, Barmina, and Frenkel, 1987). The general formats for petrochemical and geochemical datafiles used in those calculations were the basis of the current INFOREX UI. They therefore should support the existing domestic data formats and should be applicable directly to igneous petrology modeling. The INFOREX UI is hot-key driven; with function keyboard keys serving as the hot keys. The main INFOREX menu is represented by the following functions:

- F1: System Configuration
- F2: General System Information
- F3: View / Edit / Input Datafiles
- F4: Selecting Run Conditions
- F5: Setting Phase Assemblages
- F6: Exchange INFOREX Data
- F7: Developing Geothermometers

System configuration (SC) Feedback on use of the earlier versions of INFOREX showed us that working with smaller subbases is sometimes more useful than with the entire database. To make working with the subbases more convenient, we developed the settings facility. This consists of five windows (Fig. 3). One can switch between windows by using the F3 key (Next Window func.): "paths", "phases", "systems", "containers", and "filenames". Here, you can define paths to the four working subdirectories (described previously), as well as mineral, rock, and container names. All settings can be saved in a separate file to restore them whenever needed. New working sessions always begin with the last-saved settings.

General system information (GSC)

This option is implemented to obtain the number of records in the database, how they are subdivided according to presence/absence of volatiles, run duration, as well as for the purpose of browsing through all the datafiles. This information can be displayed on-screen, saved into the GENERAL.INF

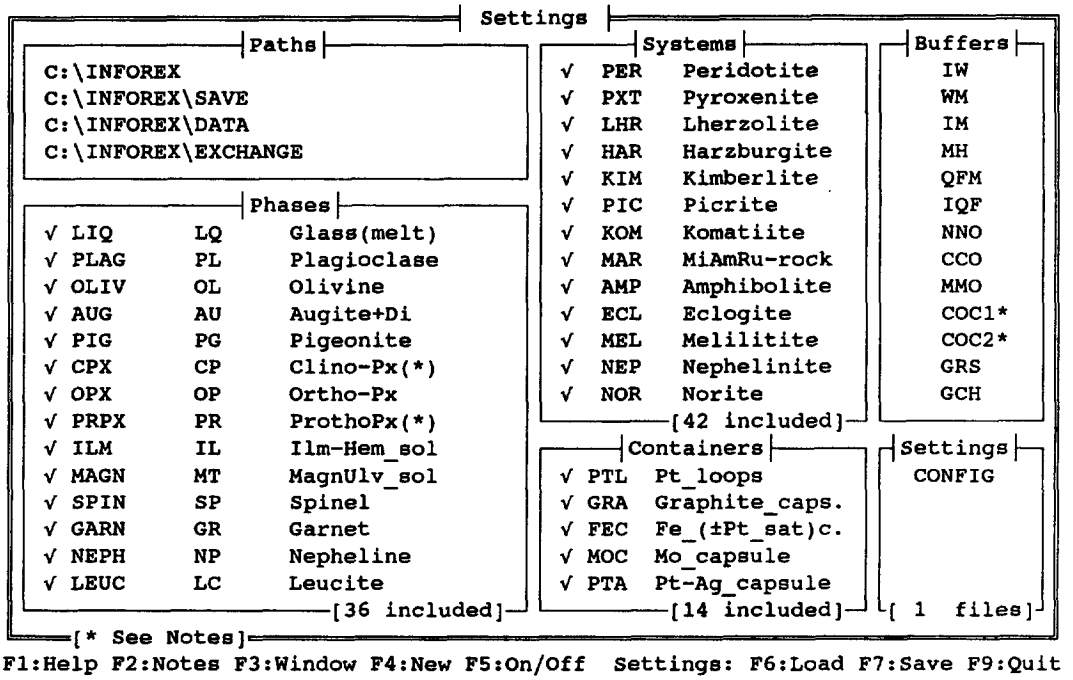

Figure 3. System Configuration option window.

file, or printed. An example GENERAL.INF file is given in Figure 4. The browse function allows the user to look through a file, and also to search any substring in the selected file. For example, one can locate an experimental investigation by a selected author in the BIBL.TXT file.

View/edit/input datafiles (VEI)

As mentioned previously, the basic database entity is an individual experimental study. The VEI option allows the user to work with the main database entities. The UI allows the user to select a particular reference. The desired object is located by scrolling page-by-page through the bibliographic records, or by selecting it at once. The number of references located while browsing can be recorded in the BIBL.TXT file using the F2 option. The UI will display the corresponding master records of CONDIT.EXP file (Fig. 5A), and all individual phase composition records linked to these masters.

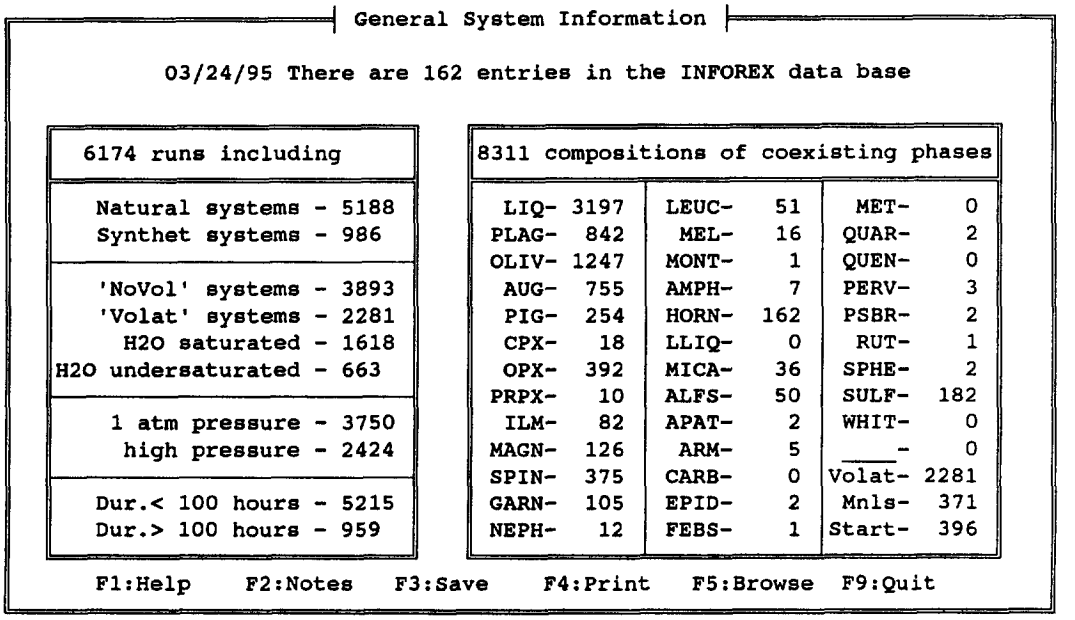

Figure 4. Window showing current state of INFOREX-3.0 database: GENERAL.INF file.

A

View of experimental data

Reference: Authors. Title //Source, Year, Vol., Numb., Pages.

Numb 31

Sack R.O., Walker D., Carmichael I.S.E. Experimental petrology of alkalic lavas: constraints on cotectics of multiple saturation in natural basic liquids//Contrib. Mineral. and Petrol., 1987, V. 96, N 1,P. 1-23.

Experimental conditions and resulted phase assemblages

N	n	SystemN/V		P,kb	Temp	lgfO2	Dur,hr	Con	Phase assemblages						
31	1	ALB - 1	N	0.0	1330	-6.77	10.0	PTL	LQ1	OL1					
	2	ALB - 1	N	0.0	1301	-7.11	10.0	PTL	LQ1	OL1	SP1				
	3	ALB - 1	N	0.0	1234	-7.93	38.5	PTL	LQ1	OL1	SP1				
	4	ALB - 1	N	0.0	1201	-8.37	100.0	PTL	LQ1	OL1	AU1	SP1			
	5	ALB - 1	N	0.0	1176	-8.72	422.0	PTL	LQ	OL	AU	SP			
	6	ALB - 1	N	0.0	1149	-9.09	217.0	PTL	LQ	OL	AU	SP			
	7	ALB - 1	N	0.0	1121	-9.51	312.0	PTL	LQ1	OL1	AU1	SP	LC1		
	8	ALB - 1	N	0.0	1064	-10.41	1460.0	PTL	LQ1	OL1	AU1	SP	SA1		
	9	ALB - 2	N	0.0	1302	-7.10	12.8	PTL	LQ1	OL1	SP				
	10	ALB - 2	N	0.0	1270	-7.48	19.3	PTL	LQ1	OL1	SP				

F1:Help F2:Notes F3:Next F4:Edit F5:Write F9:Quit PgUp/PgDn

B

Edit of experimental data

Reference: Authors. Title //Source, Year, Vol., Numb., Pages.

Numb 67

Grove T.L., Juster T.C. Experimental investigations of low-Ca pyroxene stability and olivine-pyroxene-liquid equilibria at 1-atm in natural basaltic and andesitic liquids//Contrib. Mineral. and Petrol., 1989, V. 103, N 3, P. 287-305.

Contents of major components in LIQ - phase, wt.%

Num	SiO2	TiO2	Al2O3	FeO	MnO	MgO	CaO	Na2O	K2O	P2O5	Cr2O3	H2O
1	56.20	1.27	15.20	8.76	0.19	5.43	7.80	3.42	1.16	0.19	0.05	0.00
2	57.20	1.31	14.50	8.74	0.17	4.87	7.58	3.52	1.34	0.17	0.04	0.00
3	56.90	1.59	13.90	9.15	0.21	4.49	7.53	3.55	1.43	0.22	0.03	0.00
4	57.50	1.61	14.00	8.99	0.21	4.10	7.09	3.62	1.63	0.25	0.05	0.00
5	57.40	1.74	1	9.38	0.21	3.99	6.80	3.62	1.69	0.31	0.06	0.00
6	57.70	1.75	13.90	9.41	0.17	3.69	6.79	3.75	1.77	0.23	0.03	0.00
7	57.80	1.87	13.70	9.35	0.20	3.41	6.33	3.82	1.94	0.30	0.04	0.00
8	57.30	1.97	13.60	9.63	0.19	2.99	6.21	3.96	2.23	0.33	0.10	0.00
9	58.00	2.25	13.50	9.22	0.21	2.77	5.91	3.86	2.42	0.29	0.10	0.00
10	59.40	2.32	13.40	9.35	0.17	2.66	5.50	3.74	2.60	0.43	0.00	0.00

F1:Help F2:Notes F3:Next F4:Edit F5:Write F9:Quit PgUp/PgDn

Figure 5. Window of View / Edit / Input Data Files option: bibliography for specific experimental investigation and corresponding master records in condit.exp file. A, View option display. B, Edit display (note that current working field is highlighted).

If an error is dicovered, it can be corrected in the Edit regime (Fig. 5B). When the user selects the "Input" function, the bibliographic information is requested. Then the master records are loaded (experimental conditions) as tabulated fields followed by loading weight percentages of oxides in the appropriate phase composition records. Linking these records is performed automatically. The system identifies the completed string of a master record by the first nonempty field in the phase association codenames area, and the phase composition record by one of the first three nonzero

positions so these fields must be completed. The UI does not allow incomplete data sets to be saved at present, to continue loading at another time. For large batches of data (more than 50 experiments with hundreds of microprobe analyses) we recommend either the use of the *EID*-option (see later section) or that the full set of phase associations be completed initially to inform the system about how many strings should be reserved for the phase compositions input. Then the user must input at least one of the first three columns for each phase and save this dataset. Such a "template" can be completed using the Edit function later.

Selecting run conditions (SRC)

This is one of the most important INFOREX functions oriented to petrologic applications. The *SRC*-option is implemented to perform search–match operations throughout the database according to some "filters". The groups of the filters are: the system investigated or the rock type (Earth, Lunar, Planetary, Meteoritic, Synthetic), the names of igneous rocks (basalts, komatiites, etc., see Figure 2), the combination of volatile components, experimental conditions (the range of temperatures, pressures, run durations, and oxygen fugacities), and the range of major component contents or some petrochemical ratios for the experimental glasses (if present). The screen display for presenting the *SRC* option is shown in Figure 6. After completing the search, *SRC* creates a few auxiliary files, which serve as temporary datafiles for the following procedure.

Setting phase assemblages (SPA)

Three windows appear on the screen (Fig. 7) when this option is called. In the firstwindow, all phase associations are listed that have appeared in the data subset search–matched in the (*SRC*) procedure. The second window contains a list of shortcut references to experimental investigations where these data were described. The user can exclude from these lists any phase association or an entire experimental investigation. This is convenient especially if only a single multiphase assemblage is required, for example to locate the compositions of melts equilibrated with olivine, plagioclase, pyroxenes, and spinel. When the desired arrangement is completed, the user proceeds to the third window containing the full list of phases. Here the user is asked to select two phases for further testing or for the development of mineral-melt geothermometers. The results of changes made with the *SRC* option are stored in the PROCESS.DAT file, which contains strings of CONDIT.EXP file master records as well as phase composition records of two preselected phases linked to them. The PROCESS.DAT file can be used as a temporary datafile for a mineral-melt geothermometer calculation (see *DG*-option).

Exchange INFOREX data (EID)

The *EID* option was implemented to facilitate data exchange between laboratories. We provide two functions in the data exchange option: "Export" and "Import". The first allows the user to save all the data from an experimental investigation

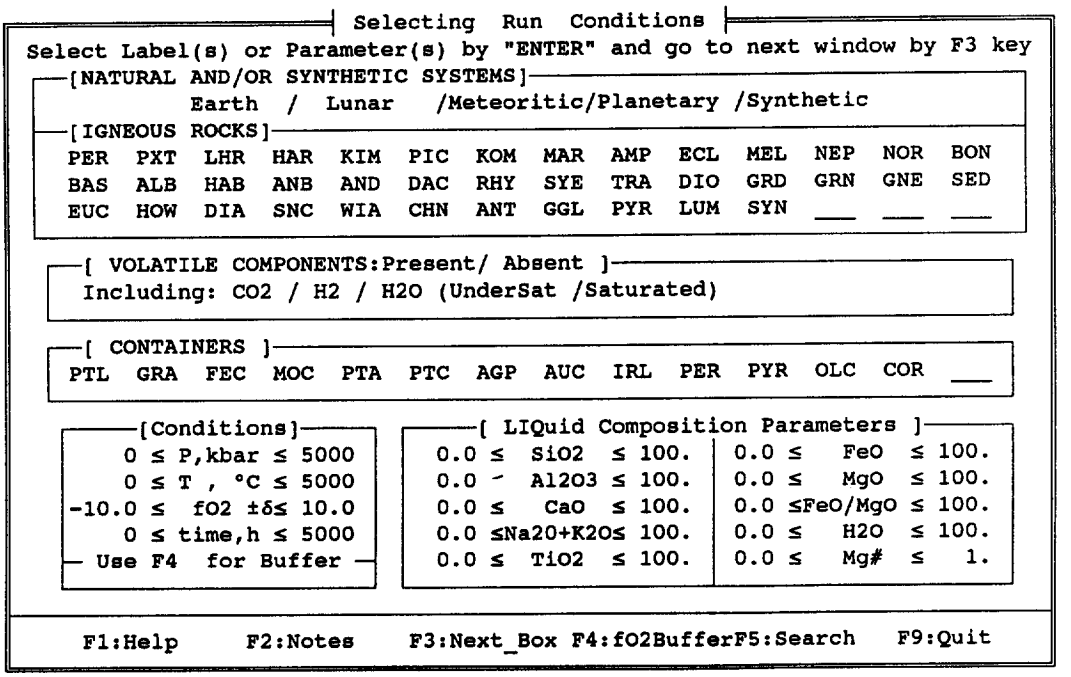

Figure 6. Window for Selecting Run Conditions option.

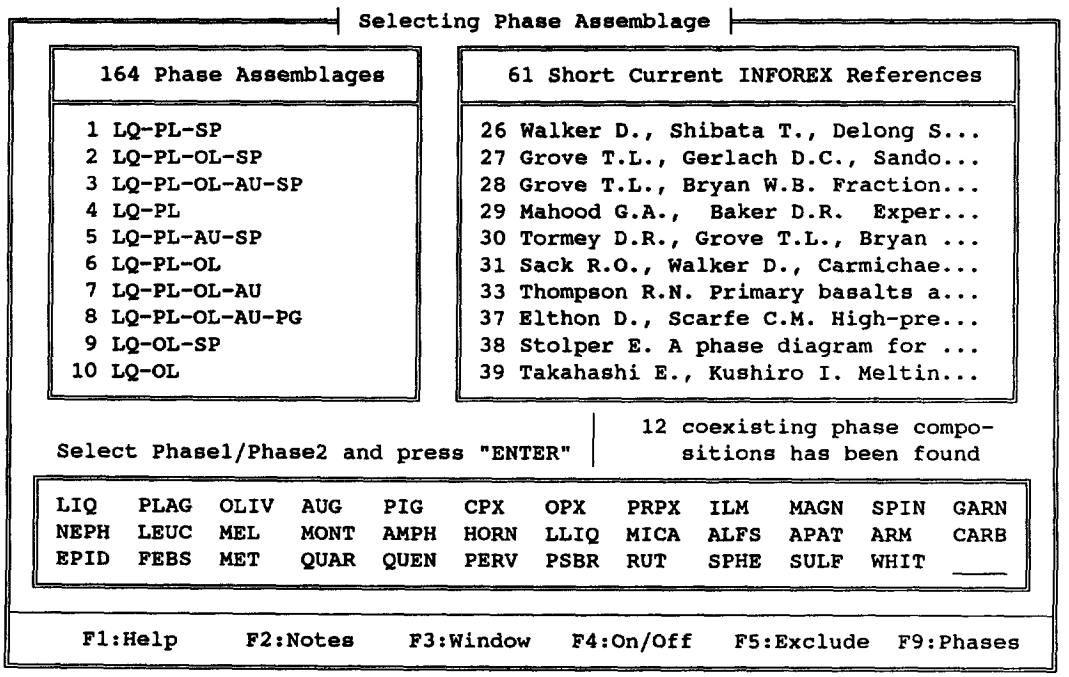

Figure 7. Window for Setting Phase Assemblages option.

to a separate file, whereas the second allows a complete dataset to be included in the INFOREX database. The exported file will appear in the...\EXCHANGE\ subdirectory and the file prepared for import must be in the same place and have.IMP extension. The following fields must be present in the records of the input file: number of the reference (the last number in your database increased by 1) in the first string, up to four next strings no longer than 73 positions—for bibliography, then word "CONDIT" followed by master records in the CONDIT.EXP file format. The next strings represent nonstandard file data (if any) in the formats of VOLAT.EXP, MNLS.EXP, and SULF.EXP files preceded by corresponding headings—VOLAT, MNLS, and SULF. Finally, strings of mineral phase compositions appear with their headings. The format of all these strings must be exactly the same as in the corresponding files of the database.

Developing geothermometers (DG)

This latest version of INFOREX system was not designed as a complete compilation of techniques for the thermodynamic processing of experimental data. Nevertheless, a set of additional INFOREX programs has been included with the system for developing empirical mineral-melt equilibria equations (geothermometers). The *DG* option creates a system of equilibrium equations if the PROCESS.DAT file includes information on low pressure olivine-melt, plagioclase-melt, pyroxene-melt (augite, pigeonite, or orthopyroxene) or spinel-melt (both chromian spinels and titanium magnetites) equilibria. Details of the processing and methods to control the accuracy of the equations are described by Ariskin and others (1996). The mineral-melt geothermometers can be used in empirical models simulating mafic magmatic differentiation processes, such as the most recent versions of the MIXFRAC program (Nielsen, 1990) and COMAGMAT programs (Ariskin and others, 1993).

HARDWARE REQUIREMENTS AND AVAILABILITY

The INFOREX-3.0 programs operate under DOS 3.0 or higher on any IBM PC compatible computer with at least 570 KB RAM and a hard disk with 2.7 MB available disk space (database files of 1.4 MB and programs of 1.3 MB). The system is distributed on either 5.25″ or 3.5″ diskettes, and is provided with an installation program; a part of the INFOREX datafiles is compressed using a domestic code. The installation procedure automatically changes the DOS AUTOEXEC.BAT file, allowing the system to be run from any directory. The INFOREX-3.0 package, including detailed documentation, is available for individuals and organizations for a fee. To obtain the system, contact Alexei A. Ariskin in the Vernadsky Institute, Moscow, Russia (*e-mail*: ariskin@glas.apc.org).

CONCLUSIONS

We believe that application of the INFOREX database in petrologic studies increases the quality and efficiency of both routine and modern tech-

niques of genetic interpretation of igneous rocks. A search of the database is fast and the requested experimental information will appear in a user-friendly form. The database can be used to accumulate and exchange experimental data between professional experimentalists, petrologists, and geochemists at all levels.

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APPENDIX 1

Examples of the INFOREX-3.0 basic data files

1. Reference source records in BIBL.TXT file:

N	Reference: Athors. Title.//Source, Year, V. ?, N ?, P. ??-??.
1	Stolper E. Experimental petrology of eucritic meteorites // Geochim. Cosmochim. Acta, 1977, V. 41, P. 587-611.

2. Master record of the CONDIT.EXP file:

N	n	Bulk Syst		P,kb	Temp	lgfO2	Dur,hr	Con	Phase assemblages						
3	7	BASL- 1	N	0.0	1156	ND	98.7	FEC	LQ1	PL	OL1	PG1	SP		
8	7	BASL+ 1	N	5.0	1200	IW*	4.0	FEC	LQ1	AU1	PG				
141	1	SYNS- 1	V	2.0	870	ND	3.0	AUC	LQ1						WS
147	1	ALB - 1	N	0.0	1200	-8.00	36.0	AGP	LQ1						RE

abbreviations see in APPENDIX 2.

3. An example of the regular phase compositions file record (such as LIQ.EXP, PLAG.EXP, SPIN.EXP, etc.).

SiO2	TiO2	Al2O3	FeO	MnO	MgO	CaO	Na2O	K2O	P2O5	Cr2O3	H2O	N	n
49.53	0.56	12.85	17.44	0.52	7.12	10.20	0.66	0.00	0.00	0.14	0.00	1	11
49.39	0.70	13.07	17.35	0.57	6.41	10.47	0.53	0.0	0.0	0.33	0.0	1	14
69.44	0.73	13.64	3.04	0.08	1.09	0.28	0.84	6.05	0.06	0.00	2.95	113	19

4. Examples of unregular phase compositions file records:

a - MNLS.EXP

N	n	An(PL)	Fo(OL)	En(AU)	Wo(AU)	En(PG)	Wo(PG)	En(OP)	Wo(OP)	__(GR)	__(GR)
89	32	.0	85.0	.0	.0	.0	.0	.0	.0	.0	.0
89	34	76.0	76.0	.0	.0	.0	.0	.0	.0	.0	.0
89	35	64.0	78.0	.0	.0	.0	.0	.0	.0	.0	.0

b - SULF.EXP

N	n	lgfS2	Melt S,wt.%	Immiscible Sulfide Liquid, wt.% S	Fe	Mn	Ni	Co	ADD	REMARKS
104	1	-1.00	0.060	00.000	00.000	00.000	00.000	00.000	00.000	
111	5	-10.24	0.028	0.000	0.000	0.000	0.000	0.000	0.000	
111	6	-3.55	0.008	37.990	61.630	0.100	0.050	0.000	0.000	

c - VOLAT.EXP

CHARGE		BULK(+sil),wt.%			BULK(+sil),mol%			BULK(-sil),mol%			X(vapor),mol%		
N	n	H2O	CO2	H2	H2O	CO2	H2	H2O	CO2	H2	H2O	CO2	H2
32	1	10.0	0.0	0.0	ND	0.0	0.0	100.0	0.0	0.0	100.0	0.0	0.0
32	2	8.8	1.8	0.0	24.0	2.0	0.0	ND	ND	0.0	ND	ND	0.0
36	1	ND	ND	0.0	ND	ND	0.0	ND	ND	0.0	25.0	75.0	0.0

d - REDOX.EXP

N	n	WT% FeO(II)	WT% Fe2O3	Mol.ratio Fe3+/Fe2+	WT% CrO(II)	WT% Cr2O3	Mol.ratio Cr3+/Cr2+	REMARKS
147	1	9.55	2.40	.226	.00	.00	.000	Fe2O3 contents were
147	2	7.54	4.82	.575	.00	.00	.000	determined by the
147	3	8.76	3.52	.362	.00	.00	.000	difference between
147	4	8.40	2.40	.257	.00	.00	.000	total iron - FeO(t)
147	5	6.50	4.60	.637	.00	.00	.000	and ferrous - FeO

APPENDIX 2

First three windows of NOTES.TXT file containing the main INFOREX abbreviations

IGNEOUS ROCK AND SYSTEM INDICATORS 1

N (No volatiles) / V (with Volatiles) / F (Fluid saturated)

\- (undozed) / + (dozed with minor or major elements, crystals, etc.)

EARTH( )/LUNAR(L)/METEORitic(M)/PLANETary(P)-Martian,Venusian/SYNTHetic(S)

1	Peridotite	-> PER	15	Basalt	-> BAS	29	Eucrite	-> EUCM
2	Pyroxenite	-> PXT	16	AlkalineBAS	-> ALB	30	Howardite	-> HOWM
3	Lherzolite	-> LHR	17	High-Al BAS	-> HAB	31	Diagenite	-> DIAM
4	Harzburgite	-> HAR	18	Andesit.BAS	-> ANB	32	Shergottite	-> SNCM
5	Kimberlite	-> KIM	19	Andesite	-> AND	33	WInc Allende	-> WIAM
6	Picrite	-> PIC	20	Dacite	-> DAC	34	Chondrite	-> CHNM
7	Komatiite	-> KOM	21	Rhyolite	-> RHY	35	ANT series	-> ANTL
8	MiAmRu-rock	-> MAR	22	Syenite	-> SYE	36	Green glass	-> GGLL
9	Amphibolite	-> AMP	23	Trachyte	-> TRA	37	Pyrolite	-> PYRS
10	Eclogite	-> ECL	24	Diorite	-> DIO	38	Lunar Mantle	-> LUMS
11	Melilitite	-> MEL	25	Granodior.	-> GRD	39	Synthetic	-> SYNS
12	Nephelinite	-> NEP	26	Granite	-> GRN	40	_____	-> ____
13	Norite	-> NOR	27	Gneiss	-> GNE	41	_____	-> ____
14	Boninite	-> BON	28	Sedimentary	-> SED	42	_____	-> ____

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NAMES OF PHASE COMPOSITION FILES AND THEIR INDECIES IN CONDIT.EXP 2

N	Phase	File	Index
1	Glass(melt)	LIQ	LQ
2	Plagioclase	PLAG	PL
3	Olivine	OLIV	OL
4	Augite+Di	AUG	AU
5	Pigeonite	PIG	PG
6	Clino-Px(*)	CPX	CP
7	Ortho-Px	OPX	OP
8	ProthoPx(*)	PRPX	PR
9	Ilm-Hem sol	ILM	IL
10	MagnUlv sol	MAGN	MT
11	Spinel	SPIN	SP
12	Garnet	GARN	GR
13	Nepheline	NEPH	NP
14	Leucite	LEUC	LC
15	Melilite	MEL	ML
16	Monticellit	MONT	MO
17	Ortho-Amph	AMPH	AM
18	Clino-Amph	HORN	HB

* see additional comments

N	Phase	File	Index
19	Second LIQ	LLIQ	LL
20	Mica (*)	MICA	MI
21	AlkFeldspar	ALFS	AF
22	Apatite	APAT	AP
23	Armalcolite	ARM	AR
24	Carbonate	CARB	CB
25	Epidote	EPID	EP
26	FeBustamite	FEBS	FB
27	Metal	MET	ME
28	Quartz	QUAR	QU
29	Quenched	QUEN	QP
30	Perovskite	PERV	PV
31	Ps-brookite	PSBR	PB
32	Rutile	RUT	RU
33	Sphene	SPHE	SH
34	Sulfide	SULF	SF
35	Whitlockite	WHIT	WI
36			

* see additional comments

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INDECIES OF CONTAINERS AND OXYGEN BUFFERS 3

Containers	Index
1 Platinum loops	PTL
2 Graphite capsule	GRA
3 Fe (±Pt sat)capsules	FEC
4 Molybdenum capsule	MOC
5 Pt-Silver capsule	PTA
6 Platinum capsule	PTC
7 Ag-Pd capsule	AGP
8 Gold capsule	AUC
9 Iridium loops	IRL
10 Peridotitic capsule	PER
11 Pyrolitic capsule	PYR
12 Olivine capsule	OLC
13 Al2O3 crucibles	COR
14 _____	___

Oxygen buffers	Index
Iron-wustite	IW
Wustite-magnetite	WM
Iron-magnetite	IM
Magnetite-hematite	MH
Quartz-Fayalite-Magn.	QFM
Iron-quartz-fayalite	IQF
Nickel -NiO	NNO
Cobalt -CoO	CCO
Mn3O4 -MnO	MMO
Graphite-CO-CO2-O2 *	COC
Graphite-CO-CO2-O2 **	COC
Graphite-COH system	GRS
Graphite-methane (ND)	GCH
_____	___

* >5 kbar, ** <5 kbar(see below)

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