Geochemistry International, Vol. 34, No. 2, 1996, pp. 85–90. Translated from Geokhimiya, No. 2, 1996, pp. 99–105.

Development of a Database on Experimental Crystal–Melt Equilibria for Igneous Rocks: INFOREX System, Version 3.0

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Received July 6, 1995

Abstract—We present the INFOREX system, which is a base of experimental data on crystal–melt equilibria of igneous rocks, and the INFOREX-3.0 data-management system. This system is designed for use in petrologic and geochemical investigations to provide fast access to experimental data and makes it possible to customize data output based on chemical criteria and the experimental conditions. The database includes 6174 experiments from 162 studies and 8311 compositions of coexisting phases. The tables of experimental conditions and the composition of run products are stored in ASCII files with fixed width fields. The main options of the INFOREX-3.0 system allow one to customize the system to work with a certain set of minerals and rocks; obtain information on the current state of the database; view, edit, and add the results of an experimental study; select experiments corresponding to a defined range of intensive parameters and mineral associations; and calculate and test geothermometers for mineral–melt equilibria. The INFOREX system can greatly enhance the efficiency of petrological and geochemical investigations and is recommended for professional petrologists as well as for university students studying geology-related fields.

INTRODUCTION

Experimental studies of phase equilibria in synthetic and natural systems that model the diversity of igneous rocks form the basis of igneous petrology. This line of investigation was started more than 70 years ago under the influence of Bowen's ideas [1], and now no genetic interpretation of the natural associations of volcanic or plutonic rocks is complete without certain experimental data. The investigation of phase equilibria in silicate systems has been developing especially rapidly since the 1970s, when the microprobe analysis of synthetic and natural minerals became a routine method in petrological investigations. This resulted in the appearance of a large body of published experimental data on the composition of coexisting minerals and quench glasses and in the formation of new avenues in igneous petrology, such as geothermometry [2] and computer simulation of magma differentiation [3–10].

A shift from accumulation of experimental data to its active use in petrological and geochemical investigations requires a thorough knowledge of the extensive literature, a qualified assessment of the reliability of data obtained, and a knowledge of methodical problems that arise during experiments carried out under various conditions. Sufficiently easy access to the available data and data screening or filtration on the basis of chemical criteria (magma composition) or experimental conditions (temperature, pressure, redox conditions) are also necessary. Furthermore, the use of modern computer-based methods to interpret igneous rocks requires the capability to independently analyze experimental data and control the accuracy of geothermometers and geobarometers developed.

This goal can be best achieved by developing a database and a convenient database-management system (DBMS) adapted for use on a personal computer. Here we present the INFOREX database and INFOREX-3.0 system specially designed to manage the database, which were developed by our group at the Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, during the last five years. In our opinion, such a system, which includes information on thousands of experiments on synthetic mixtures and igneous rock samples, is currently required in igneous petrology, and it could significantly increase the quality and efficiency of the traditional methods of petrological investigations.

CURRENT STATE OF THE INFOREX SYSTEM

At the time of the first short note on the INFOREX database, it was a system comprising 2446 experiments from 78 studies (papers, dissertations, and unpublished materials) [11]. It was an information system, rather than a search one, which we used to elaborate

our concept of database construction and the structure of data files and to specify requirements for designing experiments for given intervals of temperature, pressure, oxygen fugacity, and run duration. With this system it was possible to create files containing compositions of coexisting phases for previously selected experiments. This paper presents the latest version of the system, INFOREX-3.0 (1995), which was extended to include new experimental data (mainly accounting for the presence of volatile components) and new capabilities for manipulating the available information [12, 13]. This database currently includes 6174 experiments published in 162 studies and 8311 analyses of the phases synthesized in these experiments. The distribution of the analyses with respect to different minerals and quench glasses is shown in Fig. 1, which also demonstrates the distribution of runs depending on pressure, volatile content (water-saturated and water-undersaturated experiments), and run duration. Figure 2 demonstrates the database structure.

Description of Data Files

The data of the INFOREX database are stored as fixed width records in ASCII files. The file of literature reference, BIBL.TXT, contains a record for each experimental work in an arbitrary, user-defined order. The information on the conditions of experiments, type of rock under study (basalt, granite, norite, etc.), and experimental products (phase association) is presented in the CONDIT.EXP file. A separate file was created for each of the phases for which microprobe analyses were available, for example, olivine compositions are in OLIV.EXP. The relationships between files are defined through work numbers, run numbers for a given work, and file names for phases produced in the experiments. Note that bibliographic data in the BIBL.TXT file are given in the form required by the majority of Russian publishers; the user may also add literature references in an arbitrary format, because each of the records is a single line and is not divided into fields (year, volume, page, etc.).

The lines of the CONDIT.EXP file comprise the following fields of a fixed width: (1) work number (corresponding to the reference number in BIBL.TXT); (2) run number; (3) rock name (model composition, for example, *KOM* for komatiite); (4) number of the starting material composition (saved in the START.EXP file, if the value is not zero); (5) index for the absence (*N*) or presence (*V*/*F*) of volatile components in the system with a reference to the VOLAT.EXP file. Other fields contain values of pressure, temperature, oxygen fugacity, run duration (in hours), and an index for the type of container used in the experiment (for example, *MOC* for a molybdenum capsule). The last seven fields are designed to contain indexes of quench glasses (*LQ*) and mineral phases identified among the experimental products (for example, *SP*, chrome spinel; *PL1*, plagioclase with respective composition to be found in the PLAG.EXP file under number “1”). Except for a few cases (sulfides, metals), the compositional files are uniformly organized and include concentrations of the

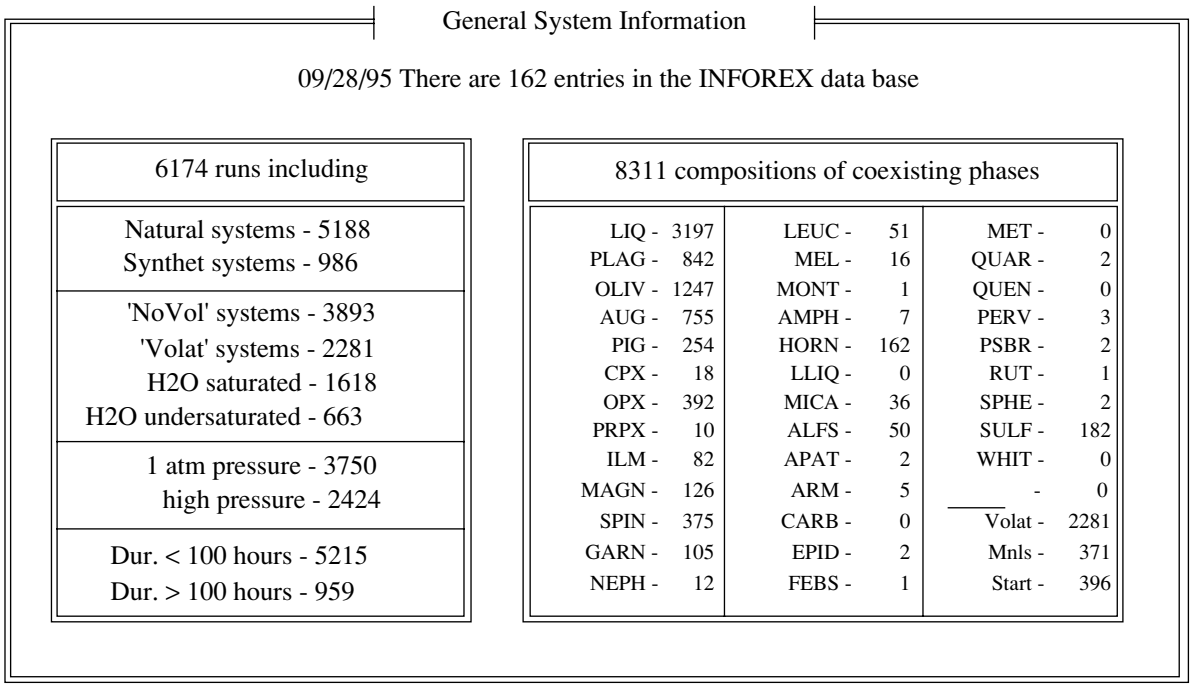

Fig. 1. Current state of the INFOREX-3.0 database.
The files of mineral compositions and the number of records in them are listed on the right side of the window (as given by the option *General System Information*).

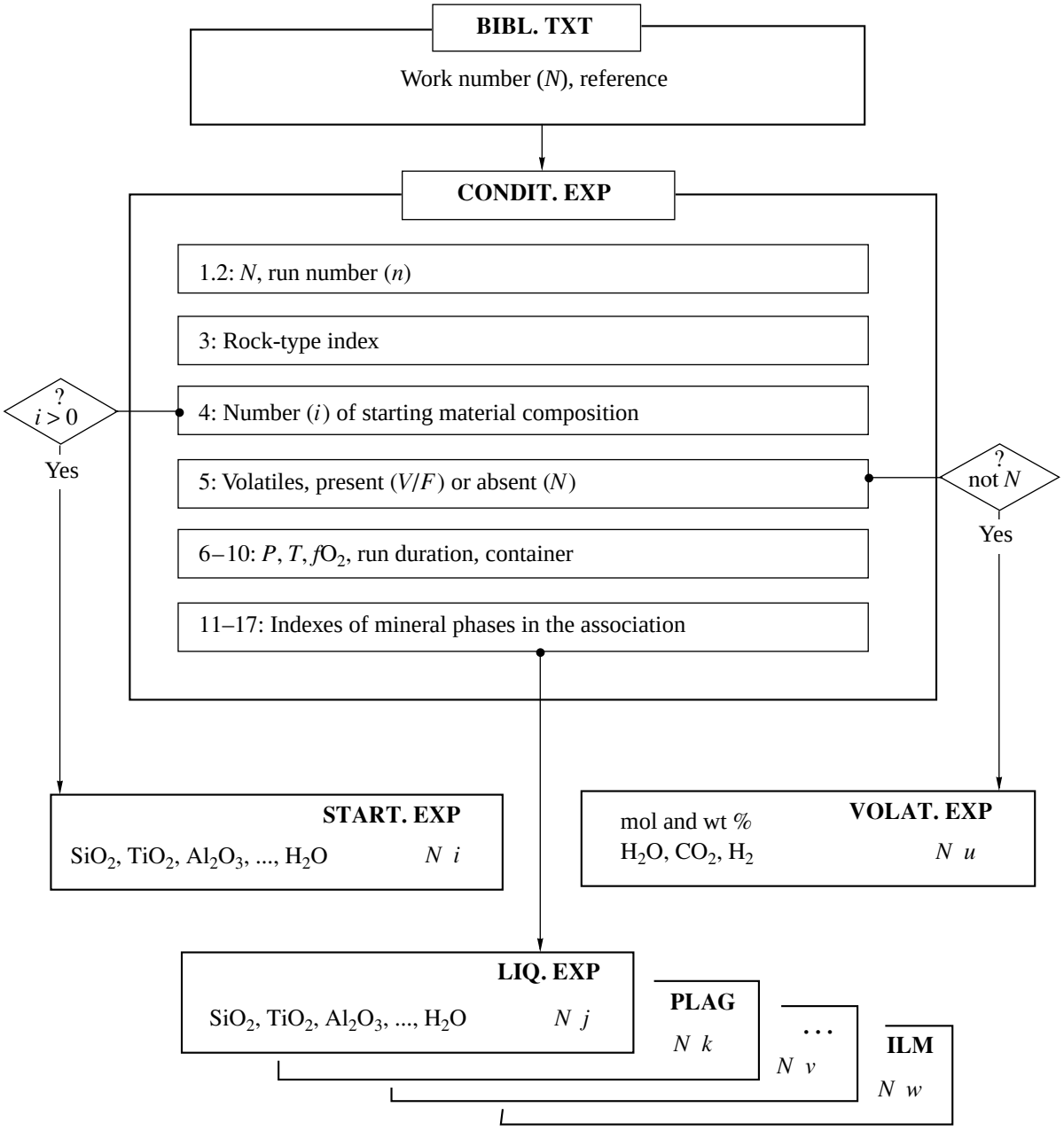

Fig. 2. Structure of the INFOREX-3.0 database.

12 major oxides in the following order: SiO_2, TiO_2, Al_2O_3, FeO, MnO, MgO, CaO, Na_2O, K_2O, P_2O_5, Cr_2O_3, and H_2O, and a reference to the respective experiment. VOLAT.EXP is an important file of a non-standard format. It includes information on experiments in water-saturated (fluid phase present, *F*) or undersaturated (*V*) conditions, such as the compositions of volatile components, and rarely, the composition of the H_2O, CO_2, or H_2 fluid phase in weight and mole percent.

The proposed system of information accumulation and storage in the INFOREX database comprises the variety of physical parameters and conditions given in the majority of experimental studies, and the order of components used corresponds to that most frequently found in the publications of petrochemical data.

DATABASE-MANAGEMENT SYSTEM INFOREX-3.0

Concept of How DBMS Handles Experimental Data

The following principles were taken as a basis for developing the database management system. First, this system should be directed at solving petrological

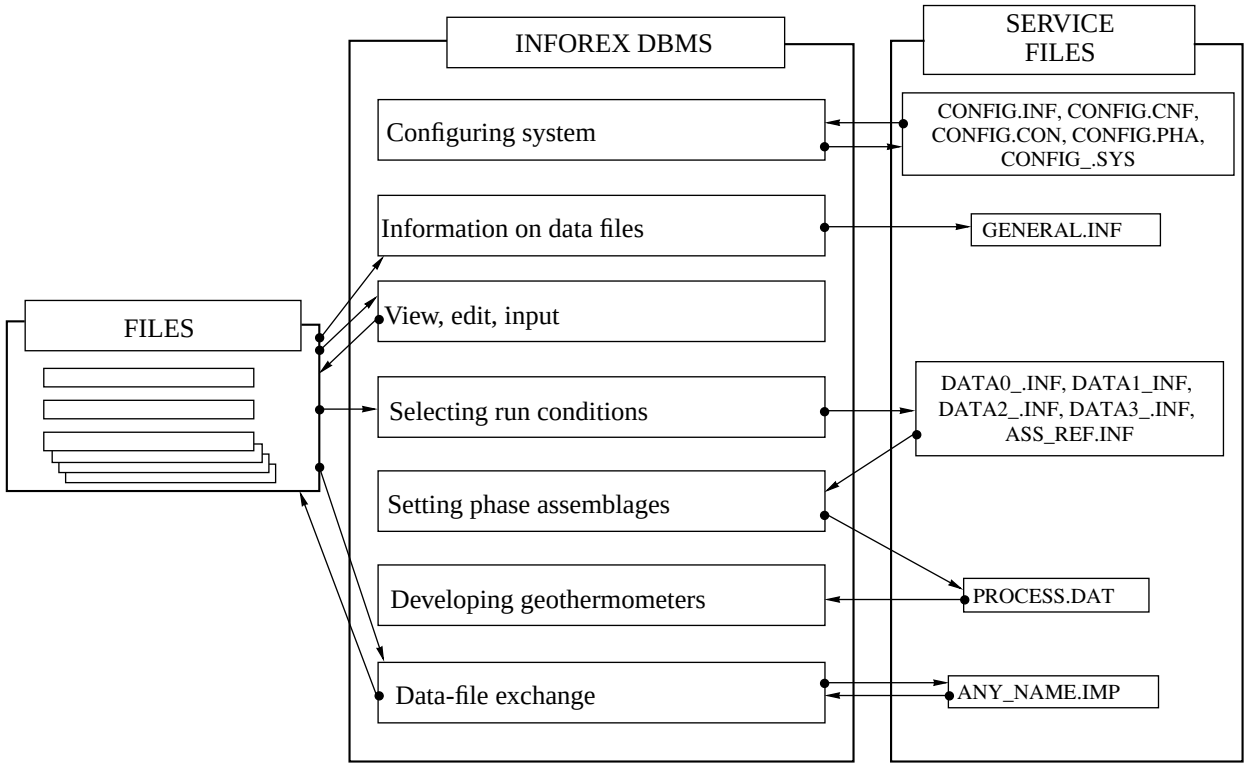

Fig. 3. Main options of the INFOREX-3.0 database-management system and the scheme of exchange between the system and data files.

problems that require experimental data on phase equilibria. This implies the development of a series of easily perceptible and convenient interfaces including generally accepted symbols and a detailed system of help pages available from any point in the program. Second, the system must provide an opportunity to correct and exchange data files accumulated by various researchers and represented in different formats. The proposed ASCII format of data files in the INFOREX system meets this requirement, as it allows corrections, creation of new files, and file exchange by using either standard editor programs or by directly interfacing with the INFOREX system in an interactive mode.

The ASCII format of data files with fixed field widths is convenient for manual editing, but the data take much more disk space compared with storage in a binary format. In addition, this somewhat slows down the search; however, these shortcomings are completely counterbalanced in modern computers by a significant increase in operating speed and disk capacity. It is possible that the general concept of data storage will be changed in further development of the database.

Let us consider the main options of INFOREX-3.0 in more detail (Fig. 3).

Configurating System[1]

The option “Configurating System” has been introduced in version 3.0 of INFOREX and is designed to define working directories, a set of mineral phases, types of rocks, and containers used for the experiments. This allows the user to divide, if necessary, the complete set of experimental data into subsystems such as high-magnesia or granite systems, which significantly accelerates search procedures and facilitates data manipulation. The transition from one subsystem to another does not require leaving the system.

General System Information

This command provides information on the current state of the database including the total number of works and experiments, the size of the condition (CONDIT.EXP) and reference (BIBL.TXT) files, the names and sizes of the mineral composition files, the number of experiments under atmospheric and high pressures, and the distribution of runs between “dry” and water-bearing systems. The information window may be sent to a printer or saved in the GENERAL.INF file (Fig. 1) in the subdirectory ...\SAVE of the INFOREX base.

[1] The names of options are given as they appear in the main menu of INFOREX-3.0 [12, 13].

The content of any file may be also viewed from the DBMS interface when information in the files is searched according to a given pattern.

View/Edit/Input

This mode is convenient for looking through the results of a particular experimental work and for creating data files containing a portion of information from it, for example, only temperatures and melt compositions. The option "Edit" allows correction of previously recorded information. Using the option "Input" is preferable for small studies, which can be input during a single work cycle in the DBMS; it reserves lines in the files of the chemical compositions of respective minerals after filling the condition file and inputting associations. The lines are automatically numbered to avoid confusion.

Selecting Run Conditions

During the information search the data are filtered in two stages, by run conditions and by liquidus phase associations. During the first stage, INFOREX 3.0 looks through the CONDIT.EXP file and selects experiments consistent with a series of user-defined parameters including: (1) the affiliation of the rocks to global systems, such as EARTH, LUNAR, METEORITE, and SYNTHETIC; (2) rock indexes, for example, only KOMATIITES, PICRITES, and BASALTS; (3) the absence or presence of volatile components including CO_2, H_2, and H_2O; (4) the container index, for example, only runs in which a platinum loop was used; (5) ranges of pressure, temperature, oxygen fugacity, and run duration; (6) restrictions on the composition of experimental glass including concentrations of major oxides—SiO_2, Al_2O_3, CaO, $Na_2O + K_2O$, TiO_2, FeO, MgO, water content (if available), and the ratios FeO/MgO (weight) and Mg# = Mg/(Mg + Fe) (mole). Records thus selected are saved in a special file, which is used in the second stage of the search.

Setting Phase Assemblages

The file created during the previous procedure has the same format as CONDIT.EXP and contains information on the phase associations and mineral–melt equilibria for a given condition range. The second stage of the search—the "Setting Phase Assemblages" option—uses this file when it is necessary to select data on the compositions of phases from a particular set of mine-rals, for example *OL–PL–LQ* or *OL–PL–AUG*.[2] This type of problem is rather common in petrological studies when a researcher needs to systematize the compositions of liquids formed by the partial melting of peridotites and equilibrated with 3–4 minerals. Another common problem is related to the analysis of data on mineral–melt and mineral–mineral equilibria for constructing geothermometers and geobarometers. On an IBM-compatible computer with a 386 or better microprocessor, INFOREX-3.0 takes several seconds to search such data. The obtained information includes the conditions of experiments and compositions of coexisting phases, which are sequentially recorded in the PROCESS.DAT file.

[2] Associations olivine–plagioclase–melt or olivine–plagioclase–augite.

Developing Geothermometers

In this version of the INFOREX system we did not pursue the goal of creating subroutines accounting for the whole variety of the methods of experimental data analysis. This can be done gradually, at the request of particular users. However, we included procedures for the development of mineral–melt geothermometers, which compose the basis of the COMAGMAT complex elaborated in our group to simulate the crystallization of basalt magmas [4]. These procedures use PROCESS.DAT as an initial file and currently allow calculation and testing of geothermometers for olivine, plagioclase, pyroxenes, and spinel [12].

Export/Import

The increasing number of INFOREX users necessitates an easy and convenient exchange of data files. It was mentioned above that the mode "View/Edit/Input" allows any portion of information to be saved in a file. The option "Export/Import" was devised to save in a file all data related to a given work (export operations) and to include experimental results prepared by other researchers into the database (import operations). It is important that an imported file strictly follow the record format, which is described in the user's manual.

CONCLUSION

The database and management system INFOREX-3.0 provides fundamentally new possibilities in the development of petrological investigations. In essence, it is a global information and search system, which can incorporate the tremendous amount of experimental data appearing each year in a great number of journals. In our opinion, such a system could become a petrological tool as important as the microscope or microprobe. Because our system makes it easy to search and process necessary information, it will ensure more efficient use of experimental data. Having such a program at hand, every researcher will be able to test and independently estimate the applicability of mineral–melt and bimineral geothermometers abundant in the petrological literature and (which is especially attractive) to learn to create them for any range of compositions and conditions.

The INFOREX system is continuously being developed. In addition to inputting new data into the database,

we plan to include programs for plotting petrochemical and phase diagrams and to start devising a version for WINDOWS. However, this version of INFOREX-3.0 is already a simple, convenient, and multitask software package, which may be used not only by petrologists but also for teaching students of geological specialities, as has been done already for several years at the Geochemistry Department of Moscow State University.

Currently, the INFOREX-3.0 data base and management system has no analogues and is a license-free product. The system takes approximately 2.5 Mbyte of disk memory (the data and programs occupy approximately equal space), and the INFOREX database management system requires approximately 570 Kbyte of RAM. The database-management system is written in the C language in the MICROSOFT QUICK-C integrated environment. The whole complex (in a partly archival form) with an installation program takes two 5.5- or 3.25-inch floppy disks. The database-management system comes with a detailed manual. Any questions on the delivery of the INFOREX system should be addressed to the authors at the Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, ul. Kosygina 19, Moscow, 117975 Russia.

ACKNOWLEDGMENTS

This work was supported by the Russian Foundation for Basic Research, project no. 94-05-16098, and the International Science Foundation, project no. M1N000.

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