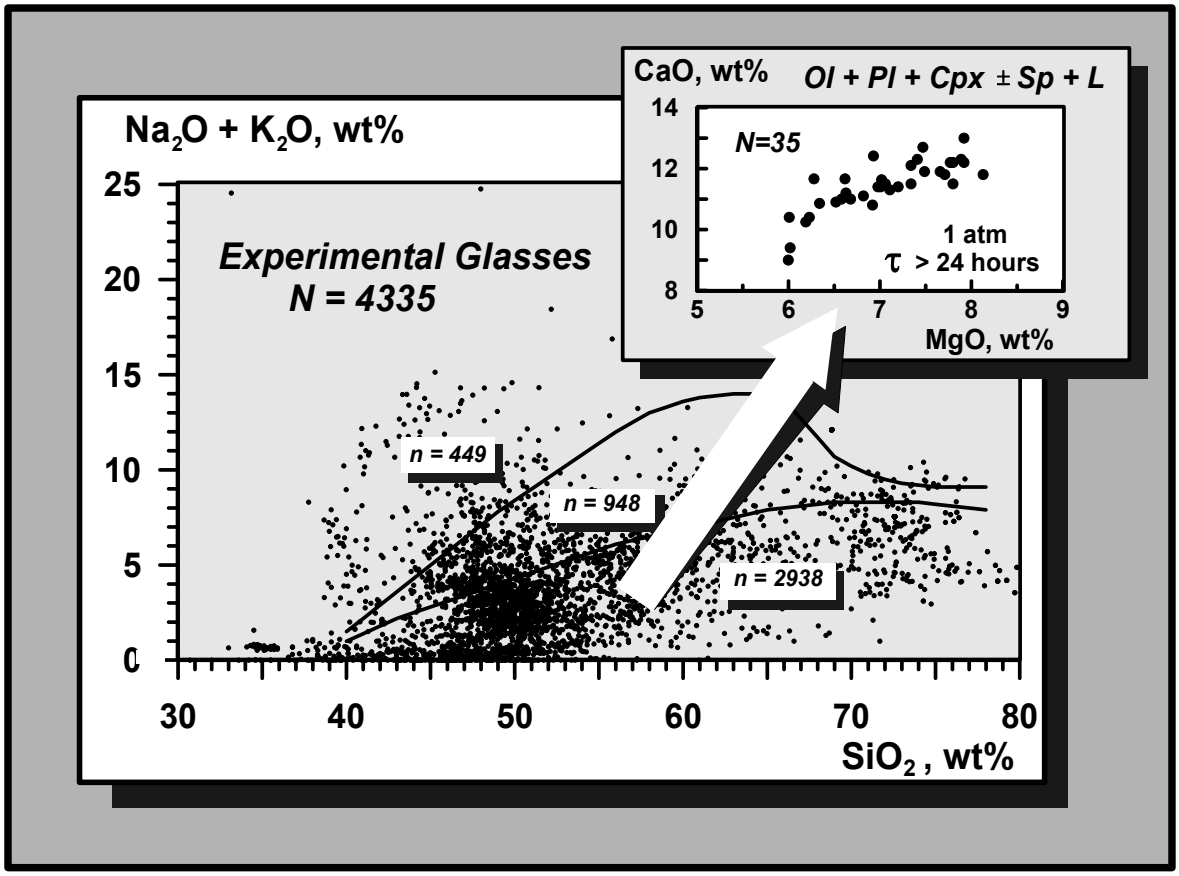
# INFOREX - 4.2 (2001)

## *Melting-Experiment Database for Igneous Petrologists and Geochemists*





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## Preface

*Welcome to the INFOREX melting-experiment database!* This is a sophisticated database manager for igneous petrologists and geochemists 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 data set, as well as to verify phase equilibria models in the field of igneous petrology.

*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 **290** experimental studies carried out from 1962 to 2000. The database includes **10,591** individual runs with **14,933** coexisting phase compositions for **44** minerals plus melt. Most of the data are based on "dry" experiments, but **4,638** 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 for the selected set of experiments; (6) export/import operations; and (7) petrological calculations, including calibrations of mineral-melt geothermometers, computations of $Fe^{3+}/Fe^{2+}$ ratios in experimental glasses, estimates of water solubility for $H_2O$-saturated experiments, and the calculations of projection parameters to plot glass compositions onto ternary diagrams.

*The INFOREX database is a powerful tool for the use in the development of petrogenetic models by providing easy access and a means for manipulating mineral-melt equilibria data*. As far as the fashion of its compositional files is same as used in COMAGMAT *(Ariskin et al., 1993; Ariskin, 1999)* and METEOMOD *(Ariskin et al., 1997b*) programs, the INFOREX database might be especially useful for petrologists who have been working with these phase equilibria models.

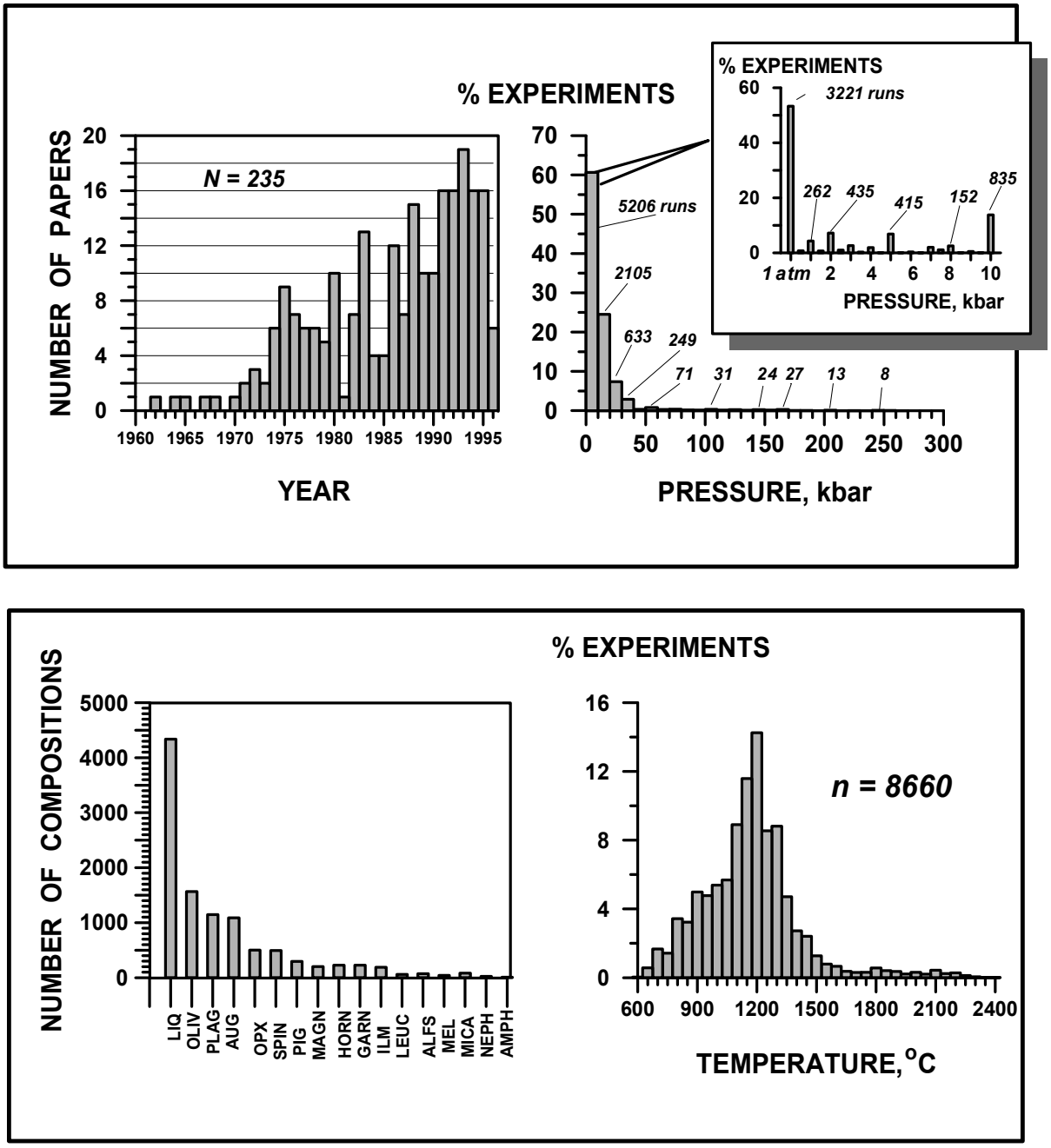



**Figure 1**. Statistics of melting-experiment information included into the main archive of the INFOREX-4.0 (1997) petrological database

*Now the system includes as much as 10,600 experiments from 290 studies*

# Chapter 1. Introduction

## *1.1. Significance of the INFOREX Database*

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 diverse 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 institutional 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 magma differentiation processes (*Nielsen and Dungan, 1983; Ariskin et al., 1987-1999; Nielsen, 1990; Weaver and Langmuir, 1990; Longhi, 1991; Ghiorso, 1995; Yang et al., 1996*).

At present, to use the available experimental data one has to laboriously navigate through the literature and evaluate the quality of the information case by case 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, select data by petrochemical criteria (igneous rock types), or run conditions (e.g., 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 et al., 1992-1997a, Meshalkin et al., 1996; Meshalkin and Ariskin, 1996*).

## *1.2. Hardware Requirements*

The main program manager, called *INFOMAN*, and other codes of the INFOREX User Interface (*UI*) were written in Microsoft C 2.5 for an IBM PC or compatible, whereas all of the *Petrological Calculation* programs were written in FORTRAN-77 with Microsoft Fortran 5 compiler. Thus, the INFOREX-4.2 programs operate under DOS 3.0 or higher on any IBM PC compatible computer with at least **1 MB RAM** and a hard disk with **7 MB** available disk space (data base files of **3 MB,** programs of **2 MB**, and a space for writing operation of **2 MB**). The INFOREX system can be succesfully used also under MS-DOS emulated from WINDOWS 95.

The system is distributed on a 3.5″ diskette and provided with an installation program; all of the the INFOREX datafiles are compressed. A hard disk drive with fast access is more critical to efficient operation. To speed up the searches and preserve your hard disk from too many writing operations one can use a virtual disk with **≈7 MB** space. The software uses SVGA monitors.

### *1.3. Availability*

Input of the melting-experiment information as well as the progamming work has been conducted by a group of scientists working at the Vernadsky Institute (Moscow, Russia): Alexei A.Ariskin, Sergei S. Meshalkin, Galina S. Barmina, Renat R.Al'meev, and Georgy S. Nikolaev were engaged in the INFOREX development process. A complete version of the INFOREX database (including the User's Manual) is distributed for a fee and can be requested from the leader of the group using the address:

**Dr. Alexei A. Ariskin**
**Vernadsky Institute, Kosygin Str. 19**
**Moscow 117975, RUSSIA**
**Fax: 7-095-938-2054, E-mail: ariskin@geokhi.ru, ariskin@rambler.ru**

## Chapter 2. General Description

In this chapter we describe the directory structure and organization of the INFOREX database files. 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 (Figs 2, 5).

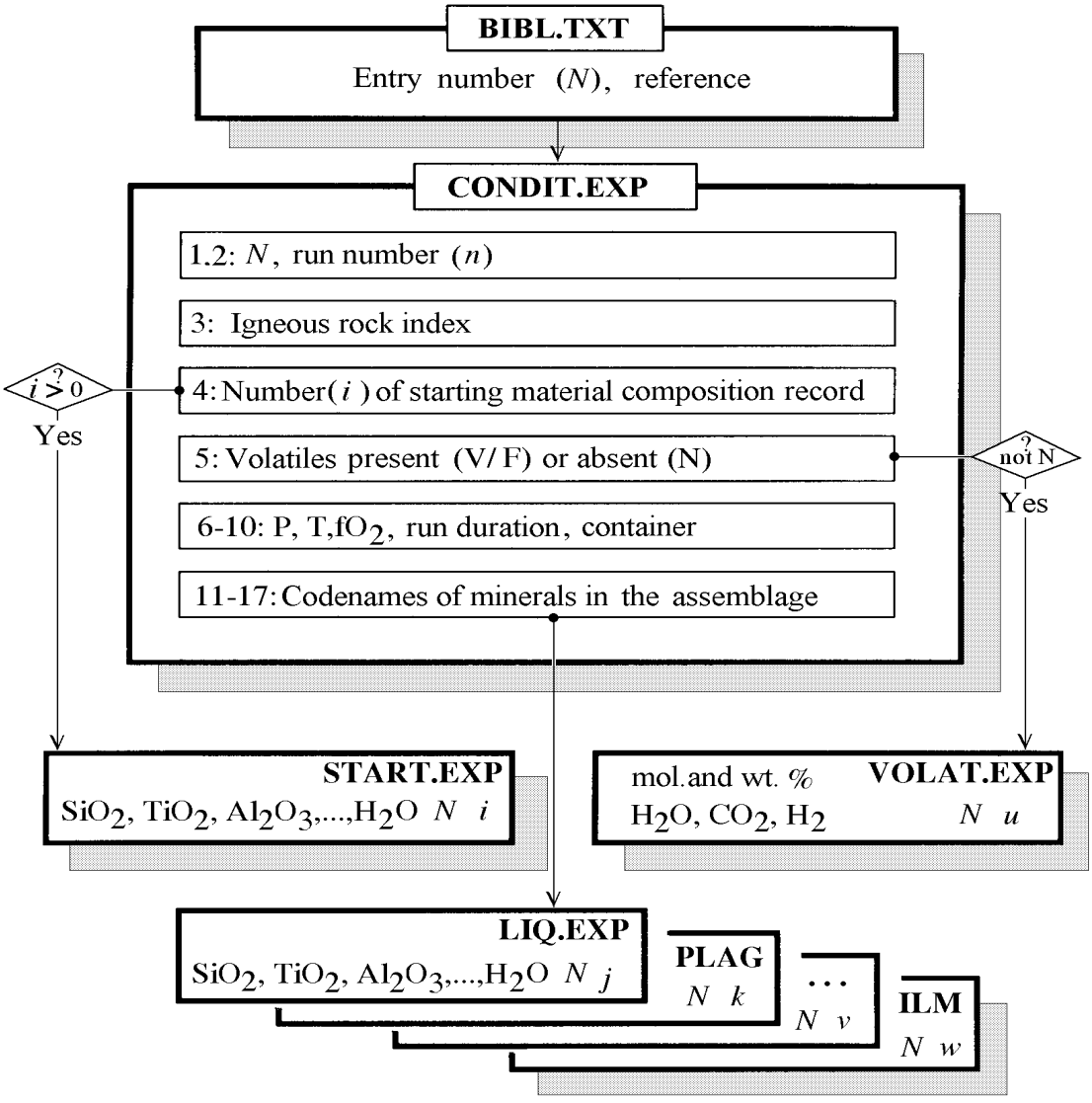



**Figure 2.** Structure of the INFOREX database files.
*The letters j, k, u, v, w denote different run numbers*

### *2.1. Database Files*

In general, the INFOREX database files can be divided into three main categories:

***basic data files,***

***data management system files,*** and

***auxiliary files***.

*The basic data files* 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 Fig. 3. *The data management system files* are designed to store information on topics 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 data files using the User Interface.

*Another group of INFOREX files* includes those formed after searching through the database or created during petrological calculations. These output INFOREX files will be discussed in a detail in *chapters 4.5-4.7*.

### *2.1.1. Structure and linkage of basic data files*

All INFOREX database files are ASCII alphanumeric rows with fixed length. The basic unit upon which the database is built is an 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 (Fig. 3). 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.

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 records of the CONDIT.EXP file:

| N | n | Bulk Syst | P,kb | Temp | lgfO2 | Dur,hr | Con | Phase assemblages | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 32 | 1 | MEL - 0 V | 30.0 | 1200 | MH* | 0.3 | AGP | LQ | OL1 | | | | |
| 34 | 1 | LHR - 1 N | 60.0 | 1850 | ND | 0.2 | GRA | LQ1 | OL2 | | | | |
| 104 | 1 | BAS + 0 N | 0.00 | 1200 | -10.98 | 48.0 | COR | LQ1 | PL | OL | SF | | |
| 111 | 1 | AND + 1 F | 2.0 | 800 | -14.18 | 102.0 | AUC | LQ1 | PL1 | SF1 | CP | HB | |
| 124 | 1 | KIM - 1 V | 10.0 | 1400 | ND | 0.2 | PTC | LQ | OL2 | | | | |
| 147 | 1 | ALB - 1 N | 0.0 | 1200 | -8.00 | 36.0 | AGP | LQ1 | RE | | | | |
| 149 | 8 | BAS + 0 N | 0.0 | 1202 | -8.01 | 17.5 | PTL | LQ1 | OL | RE | | | |
| 211 | 7 | CHAR- 2 V | 6.9 | 925 | ND | 168.0 | AUC | LQ1 | PL2 | AF | OP2 | IL | MT | AP |
| 226 | 1 | RHY - 1 F | 0.8 | 850 | NNO+1.0 | 144.0 | PTC | LQ1 | WS | | | | |
| 231 | 43 | RHY - 2 V | 1.0 | 1075 | NNO | 25.0 | AGP | LQ1 | RE | | | | |
| 232 | 2 | DIO - 1 V | 6.9 | 950 | ND | 96.0 | AUC | LQ | PL2 | AF | OP2 | GR2 | SP | * |

3. Records of a regular phase composition file (LIQ.EXP):

| SiO2 | TiO2 | Al2O3 | FeO | MnO | MgO | CaO | Na2O | K2O | P2O5 | Cr2O3 | H2O | N | n |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 46.30 | 0.18 | 4.80 | 8.90 | 0.17 | 32.90 | 4.40 | 0.46 | 0.00 | 0.00 | 0.00 | 0.00 | 34 | 1 |
| 56.81 | 2.47 | 18.50 | .88 | .00 | 7.61 | 7.97 | 3.10 | 1.16 | 0.00 | 0.00 | 0.00 | 104 | 1 |
| 64.80 | 0.20 | 15.11 | 1.90 | 0.11 | 0.15 | 1.59 | 4.52 | 5.15 | 0.00 | 0.00 | 6.02 | 111 | 1 |
| 47.08 | 3.02 | 15.90 | 11.71 | 0.16 | 6.14 | 10.71 | 2.86 | 0.86 | 0.48 | 0.00 | 0.00 | 147 | 1 |
| 47.99 | 1.96 | 15.09 | 11.07 | 0.28 | 5.84 | 8.28 | 3.07 | 4.75 | 0.00 | 0.00 | 0.00 | 149 | 8 |
| 72.92 | 0.31 | 14.56 | 1.82 | 0.08 | 0.37 | 0.89 | 2.58 | 6.17 | 0.33 | 0.00 | 0.00 | 211 | 7 |
| 77.70 | 0.07 | 13.00 | 0.38 | 0.04 | 0.05 | 0.52 | 4.08 | 4.19 | 0.00 | 0.00 | 1.88 | 226 | 1 |
| 77.30 | 0.13 | 12.42 | 1.03 | 0.03 | 0.05 | 0.35 | 4.12 | 4.53 | 0.00 | 0.00 | 6.80 | 231 | 1 |

4. Examples of records of irregular phase compositions files:

*a* - 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 |
| 124 | 1 | 6.2 | 4.8 | 0.0 | ND | ND | 0.0 | 76.0 | 24.0 | 0.0 | ND | ND | 0.0 |
| 226 | 1 | ND | ND | 0.0 | 3.0 | ND | 0.0 | ND | ND | 0.0 | 32.0 | 68.0 | 0.0 |

*b* - MNLS.EXP

| N | n | An(PL) | Fo(OL) | En(AU) | Wo(AU) | En(PG) | Wo(PG) | En(OP) | Wo(OP) | __(GR) | __(GR) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 34 | 1 | .0 | 94.4 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 211 | 7 | 32.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 53.0 | 0.6 | 0.0 | 0.0 |
| 232 | 2 | 36.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 38.0 | 1.0 | 72.0 | 24.0 |

*c* - 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 | 1 | -3.32 | 0.020 | 37.810 | 61.070 | 0.090 | 0.030 | 0.000 | 0.000 | |

*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=1.111(FeOt-FeO) |
| 149 | 8 | 8.80 | 2.51 | .257 | .00 | .00 | .000 | 5% Ol present |
| 231 | 43 | 0.88 | 2.61 | 2.669 | 0.00 | 0.00 | 0.000 | |

**Figure 3.** Examples of the INFOREX-4.2 (2001) basic data files

Usually this run number corresponds to the sequence of run conditions and phase assemblages given in tables in the source, but this sequence has been changed

in cases where retention of the original numbers would have caused difficulty in the manipulation of the data.

*The CONDIT.EXP master file records* (Figs 2 and 3.2) include essential information about each run, such as: (1) the type of igneous rock or synthetic system, (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/fluid saturated experiments and **V** - only undersaturated with volatiles runs). These switches refer the user to the VOLAT.EXP file (Fig. 3.4.*a*). Other important information fields are total pressure, temperature, oxygen fugacity, run duration, and up to 7 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 the ".EXP" extensions (see *Appendix 1*). These files (Fig. 3.3) contain records formatted as 12 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: $SiO_2$, $TiO_2$, $Al_2O_3$, $FeO_{tot}$, 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. 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 (minus silicates) as well as the volatile component contents in a vapor phase for fluid-saturated experiments (if present) - Fig. 3.4.*a*.

The second irregular file shown in Fig. 3.4.*b* 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 was 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 we will not lose even this rudimentary experimental information, 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 (see Fig. 3.2).

Two more irregular files are SULF.EXP and REDOX.EXP. The first one (Fig. 3.4.*c*) can contain weight percent S, Fe, Mn, Ni, and Co - the components of majority of sulfide phases (if present). The second file (Fig. 3.4.*d*) 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.

### *2.1.2. Data management system files*

The core of the INFOREX database is composed of three kinds of system files:

1) files containing information on the INFOREX environment, including the general directory structure, run products configuration and searching control system,

2) HELP.TXT file responsible for the on-line INFOREX help, and

3) a file called NOTES.TXT that clears the main INFOREX abbreviations, being simultaneously linked with the INFOREX *System Configuration* option (see *chapter 4.1*).

*The main environment file* **CONFIG.INF** is located in the INFOREX root directory and consists of one record describing the current operating session ...\DATA subdirectory, e.g.:

***D:\INFOREX\DATA.97***

In the D:\INFOREX\DATA.97\ 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:

***D:\INFOREX***
***D:\INFOREX\SAVE***
***D:\INFOREX\DATA.97***
***D:\INFOREX\EXCHANGE***

```
CONFIG.SYS file (STANDARD)
√   PER    Peridotite
√   PXT    Pyroxenite
√   LHR    Lherzolite
√   HAR    Harzburgite
√   KIM    Kimberlite
√   PIC    Picrite
√   KOM    Komatiite
√   MAR    MiAmRu-rock
√   AMP    Amphibolite
√   ECL    Eclogite
√   MEL    Melilitite
√   NEP    Nephelinite
√   NOR    Norite
√   BON    Boninite
√   BAS    Basalt
√   ALB    AlkalineBAS
√   HAB    High-Al_BAS
√   ANB    Andesit.BAS
√   AND    Andesite
√   DAC    Dacite
√   RHY    Rhyolite
√   SYE    Syenite
√   TRA    Trachyte
√   DIO    Diorite
√   GRD    Granodior.
√   GRN    Granite
√   GNE    Gneiss
√   SED    Sedimentary
√   EUC    Eucrite
√   HOW    Howardite
√   DGN    Diogenite
√   SNC    Shergottite
√   WIA    WIncAllende
√   CHN    Chondrite
√   ANT    ANT_series
√   GGL    Green_glass
√   PYR    Pyrolite
√   SYN    Synthetic
√   MNT    Aug_Minette
√   TON    Tonalite
√   CHA    Charnockite
√   ___    ___________
```

These working directory pointers provide the user with the flexibility necessary to be able to simultaneously work 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**). The number of names given in these files is not limited, while the current configuration given in the NOTES.TXT file supports exactly **14** different containers, **36** mineral phases, and **42** rock types. Thus, by using this specific configuration program option (see *chapter 4.1*) one can automatically customize the INFOREX system to work with any dataset.

The D:\INFOREX\DATA.97\ directory contains also a binary **SEARCH.CNF** file to store a current information on the searching configuration.

**CONFIG.PHA file (STANDARD)**

| | | |
|---|---|---|
| √ LIQ | LQ | Glass(melt) |
| √ PLAG | PL | Plagioclase |
| √ OLIV | OL | Olivine |
| √ AUG | AU | Augite+Di |
| √ PIG | PG | Pigeonite |
| √ CPX | CP | Clino-Px(*) |
| √ OPX | OP | Ortho-Px |
| √ PRPX | PR | ProthoPx(*) |
| √ ILM | IL | Ilm-Hem_sol |
| √ MAGN | MT | MagnUlv_sol |
| √ SPIN | SP | Spinel |
| √ GARN | GR | Garnet |
| √ NEPH | NP | Nepheline |
| √ LEUC | LC | Leucite |
| √ MEL | ML | Melilite |
| √ AMPH | AM | Ortho-Amph |
| √ HORN | HB | Clino-Amph |
| √ MICA | MI | Mica_(*) |
| √ ALFS | AF | AlkFeldspar |
| √ APAT | AP | Apatite |
| √ ARM | AR | Armalcolite |
| √ CARB | CB | Carbonate |
| √ EPID | EP | Epidote |
| √ ALSI | AS | Alumina-sil |
| √ QUAR | QU | Quartz |
| √ PERV | PV | Perovskite |
| √ PSBR | PB | Ps-brookite |
| √ SULF | SF | Sulfide |
| √ CAPV | Pc | Ca-perovsk |
| √ MGPV | Pm | Mg-perovsk |
| √ TOUR | TU | Tourmaline |
| √ CRND | CO | Corundum |
| √ ZRCN | ZR | Zircon |
| √ MONT | MO | Monticellit |
| √ RUT | RU | Rutile |
| √ SPHE | SH | Sphene |
| - CORD | CD | Cordierite |
| - STRL | ST | Staurolite |
| - MNZT | MZ | Monazite |
| - QUEN | QP | Quenched |
| - FEBS | FB | FeBustamite |
| - MET | ME | Metal |
| - LLIQ | LL | Second_LIQ |

**CONFIG.CON file (STANDARD)**

| | | |
|---|---|---|
| √ PTL | Pt_loops | |
| √ GRA | Graphite_caps. | |
| √ FEC | Fe_(±Pt_sat)c. | |
| √ MOC | Mo_capsule | |
| √ PTA | Pt-Ag_capsule | |
| √ PTC | Pt_capsule | |
| √ AGP | Ag-Pd_capsule | |
| √ AUC | Gold_capsule | |
| √ IRL | Iridium_loops | |
| √ PER | Peridotite_cap | |
| √ COR | Al2O3_crucible | |
| √ REC | Rh_capsule | |
| √ PRH | Pt-Rh_capsule | |
| √ AUP | Au-Pd_capsule | |
| - CUC | Cu_capsule | |

*File HELP.TXT* was designed to support on-line help in the data management system (see *Appendix 1*). It is located in the main INFOREX directory and is written in the rigorously defined format so we do not recommend changing anything in the file.

The user can get help anywhere in the UI using [***F1***] key. “Help” informs you how to work with the data management system, explains assignements of all active keys in option windows. You can scan the information by [***PgUp***] and [***PgDn***] keys; beep signals mean you are at the top or bottom of the HELP.TXT file.

To return to the user interface you should press [***Esc***] key (see prompt at the left bottom angle).

*File NOTES.TXT* explains all abbreviations of INFOREX database files (see *Appendix 1*). It contains codenames for igneous rocks and systems, names of phase composition files and their codenames in CONDIT.EXP file, abbreviations for containers and oxygen buffers, parameters of oxygen buffers equations describing temperature and pressure dependence of oxygen fugacity, as well some additional comments.

You can navigate through the on-line “Notes” exactly as through the “Help” except the calling key is [***F2***] instead of [***F1***]. One should not change the NOTES.TXT file.

*2.1.3. Auxiliary files*

The auxiliary files facilitate the manipulation of data and data swapping among the basic data files using the UI. Usually, the auxiliary files are deleted after each working session, but some of them are stored and overwrited during other sessions.

Few examples of the most important auxiliary files are listed in Table 1 and will be discussed in detail in the following chapters.

**Table 1.** The most important auxiliary files

| File Name (s) | Initially present | Creating Option | After Work |
|---|---|---|---|
| DATA0_.INF<br>DATA1_.INF<br>DATA2_.INF<br>DATA3_.INF<br>ASS_REF.INF | NO | *SRC* | Overwrited |
| # | NO | *SRC* | Overwrited |
| BASE.ERR | NO | *SPA* | Overwrited |
| DATA2_.)$(<br>DATA3_.)$( | NO | *SPA* | Deleted |
| PROCESS.CNF<br>PROCESS.DAT<br>COEXIST.DAT<br>REGRESS.OUT | NO | *Mineral-Melt Geothermometers* | Overwrited |
| FE2FE3 | NO | *Fe3+/Fe2+ ratios* | Deleted |
| H2OMODEL | NO | *Water Solubilty* | Overwrited |
| TERNARY | NO | *Ternary Diagrams* | Overwrited |

### *2.3. Directory structure*

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 called INFOMAN.EXE as well as some management system files. Basic experimental data files, BIBL.TXT file and configuration files are located in the *D*:\INFOREX\DATA\.. subdirectory.

Two other subdirectories called *D*:\INFOREX\EXCHANGE\ and *D*:\INFOREX\SAVE\ begin as empty ones after installation. The first one is created for the *IMPORT/EXPORT* operations (*Exchange INFOREX Data* option), which provide an easy exchange of the experimental data files between different users.

The second subdirectory serves mainly to store datafiles resulted from the searching through the INFOREX database (e.g., files in the PROCESS.DAT fashion), as well as output files incuding results of thermodynamic processing and some other petrological calculations. The GENERAL.INF file (see comments to Fig. 6) and files created to store configurations of searching throughout the INFOREX database (*.SEL) will be also placed into the *D*:\INFOREX\SAVE\.. directory.

*Users can change the names of these subdirectories, but must keep its general structure intact*.

## Chapter 3. Setting Up INFOREX

The *Setting Up* procedures include installation, start and configuration of the INFOREX system. During the installation one should create a directory structure and transfer properly all of the working files to a hard disk (*for this purpose we provide an installation program*). After installation and running INFOREX, if necessary, one can change a standard configuration of the database, icluding modifications of igneous rock indicators, set of minerals, etc. (see *chapter 4.1*).

**Note: At least 1 MB free conventional memory should be available on your computer to work properly with the INFOREX-4.2 database (*see Troubleshooting*).**

**Before installation of the INFOREX system, make sure that the disk you are going to install INFOREX on does not contain the directory ..\INFOREX. If this subdirectory exists on the disk, rename or remove it.**

*Installation*

To install INFOREX on your hard disk, insert your floppy disk ***INFOREX*** in drive A or B, make it active and type in the command line:

**INSTALL *D*:**

where *D* is drive letter (C, D, E...); note the space between INSTALL and the hard disk name, and colon sign after the name.

The installation program begins to create the INFOREX directory structure and to transfer the system files into the above mentioned subdirectories. After the installation is completed, pull out the floppy disk and start INFOREX.

*Starting INFOREX*

To start the INFOREX database you should run the main program manager called INFOMAN.EXE located in the main *D*:\INFOREX\.. directory. Make the *D*:\INFOREX\ directory the current one, type in the command line **INFOMAN** and press "Enter".

## Chapter 4. Description of User Interface

If you first started INFOREX you were find yourself in the **Main Menu** window, including 7 main INFOREX options (Fig. 4). All of the options can be called by pressing the [***F1***] to [***F7***] keys, provided the INFOREX User Interface is hot-key driven, with function keyboard keys serving as the hot keys. Detailed descriptions of working sessions with the functions are followed below.

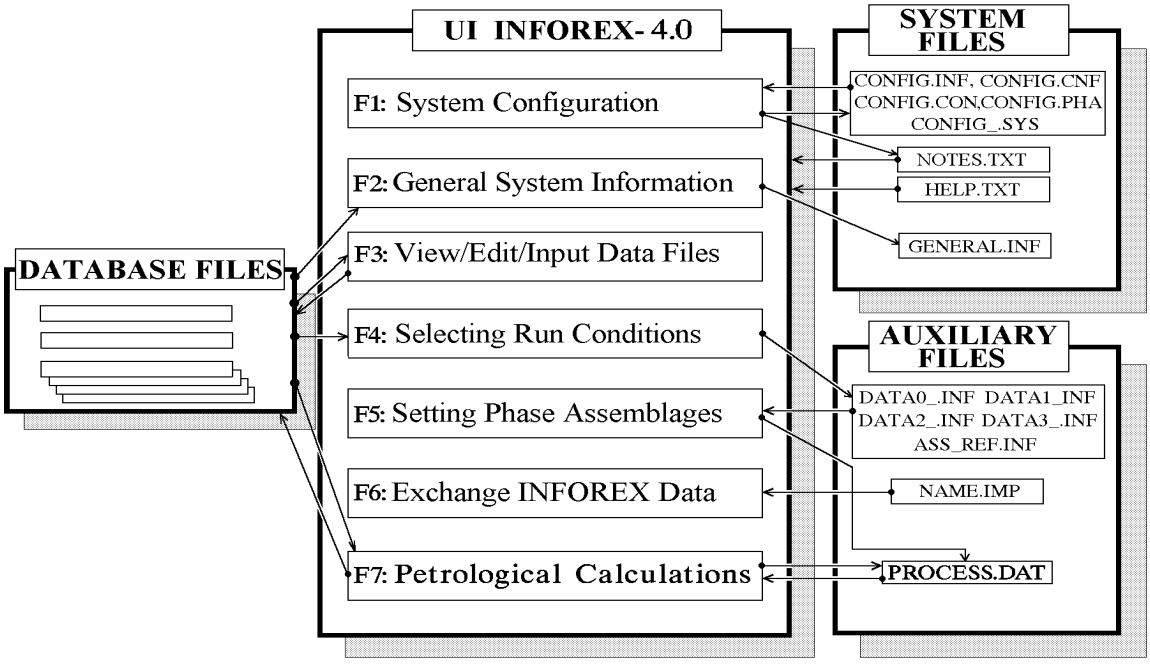



**Figure 4**. Structure of the INFOREX-4.2 (2001) data management system

**Note:** **To scroll through a page (*frame or window*) corresponding to a selected *Main Menu* option one should use the arrow keys, whereas for going to another page within a function use the [*PgUp*] and [*PgDn*] keys.**

**Press the [*Shift*]+[*F3*] keys, if you want to come back to the initial screen or to a previous window.**

### *4.1 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. Moreover, it was necessary to develop a facility which allows users to change or to input new mineral abbreviations, igneous rock or synthetic system indicators, indecies of other oxygen buffers and containers. To address all of the problems *the System Configuration option* has been developed.

**Note:** **This option has been developed for users experienced in the practical applications of the INFOREX system. Therefore, at an initial stage of using the INFOREX we strongly recommend starting with a standard INFOREX configuration provided during the installation process (see *chapter 3.1*).**

So, if you are already familiar with the INFOREX system and really need to reconfigure the database, run INFOREX and press [***F1***] key to choose the *SC* option from the *Main Menu*.

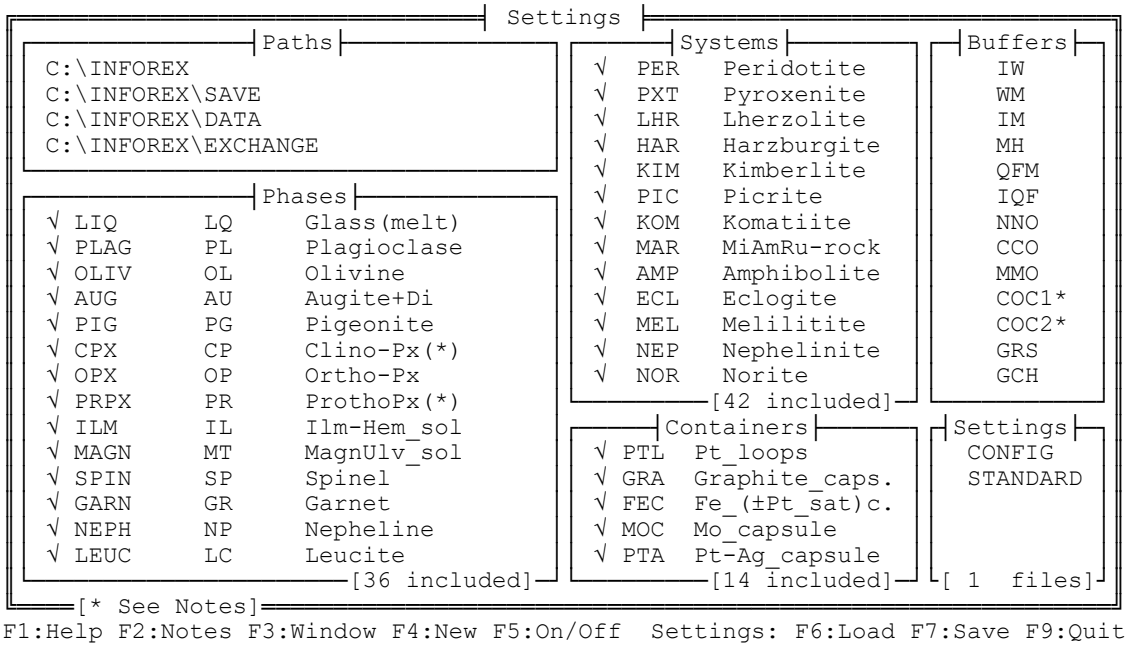



**Figure 5**. Screen image of the **System Configuration** option

A screen image will appear at your monitor (Fig. 5), including five windows "*Paths*", "*Phases*", "*Systems*", "*Containers*", and "*Settings*" which could be edited during a reconfiguration, as well as the "*Buffers*" window just demonstrating the oxygen buffers included. One can switch between the windows using the [***F3***] (***Window*** - *Go Forward*) or [***Shift***]+[***F3***] (*Go Backward*) keys.

**Note: For all but EXCHANGE INFOREX DATA functions the use of the [*F1*], [*F2*] and [*F9*] keys is similar:**

**[*F1*] (*HELP*) provides the on-line help which displays and comments all specific options of INFOREX-4.2 (2001); [*F2*] (*NOTES*) involves 5 pages with tables deciphering indicies, search words and flags used in the database; [*F9*] (*QUIT*) quits the current operation.**

*Paths* window

This is the first active window of the *SC* option designed to define paths to the four working INFOREX subdirectories (see *Directory structure*). To make some changes, just type the new ones over the default paths and press "Enter". Go up and down (*only if you are no typing a new path !*) within the window by [↑] or [↓] keyboard keys.

*Phases* window

To get this window, just press the [***F3***] key. Now you can add a new mineral phase name in the default set or replace an existing one with another. To do this you should first disable an old mineral phase name (in which you probably do not need during a forthcoming work with INFOREX). It is necessary to do this because the current version of INFOREX-4.2 requires that the total number of *phases* should not exceed 36 for each working session.

So, choose the name to disable and press the [***F5***] (***On/Off***) key. As a result, the enable flag (√) disappear and the number in the lower right corner of the window is decreased by one. After that press the [***F4***] (***New***) key to call input fields as follows:

```
Enter file name, short name, and commentary
          for the new phase:
   TEST      TS     Testing-PHA
```

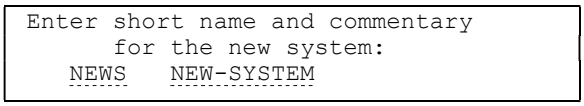
Type sequently the name of a new file where microprobe data for the new phase will be stored (3-4 symbols, *e.g. TEST*) and a short name of this phase which will be referred to (exactly 2 symbols, *e.g. TS*), followed with a commentary (usually a complete mineral name, up to **11** symbols).

**Note: the commentary both here and within the other windows *must be* an inseparatable single word (use "_" or "-" symbols to connect separate words, *e.g. Testing-PHA*).**

After completing the operations the new phase name will appear in the list of phases just after the old name is disabled. You can change any number of default names in a similar fashion: *monitor the total number in the lower right corner which should be equal to 36.*

*Systems* window

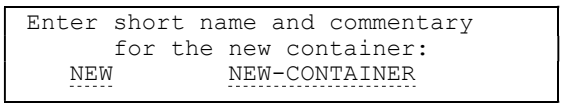
To get the window press the [***F3***] (***Window***) key again. Here, one can create a new rock type or synthetic system indicators with a commentary (usually, a complete name of igneous rock or a commonly used silicate system abbreviation, up to **11** symbols). All of the input operations are absolutely the same as for the *Phases* window - the input fields look like the following:




**Note: the length of the new system name must be 3 or 4 symbols, whereas the total number of system indicators should not exceed 42.**

*Containers* window

This window is designed to display or to change the working set of containers included into INFOREX-4.2 database. Container materials are known to be an important feature of experimental conditions, because they can control oxygen fugacity or change the bulk chemical composition of the initial charge. To allow users to filter experimental data based on the materials, we have included in the database a list of commonly used containers (see NOTES.TXT in *Appendix 1*). If there is a need to input a new container name, you should follow the rules as described above. Two input fields are shown in the screen message:

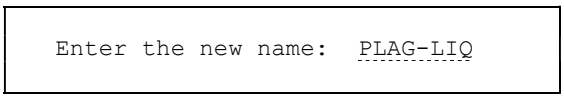



Keep in mind that the input field for the container name is of exactly 3 symbols, whereas the commentary field can contain up to **14** symbols. The total number of containers must also be equal to **14**.

*Settings* window

This window is designed to save your custom settings to a separate file or load into INFOREX previously saved settings.

*To save* your new settings press the [***F7***] (***Save***) key. If you are going to save the settings as a new file, press [***F4***] (***New***) and type the new name (*without extension!*) in the frame that will appear in the screen:




and press “Enter”. If you wish to store the settings in a file that already exists on the disk, select this file (turn the enable flag of the selected file name on and that of other file names - off by the [***F5***] key) and press the [***F7***] key again.

**Note: all of the changes described above are always written directly into the family of INFOREX configuration files (CONFIG.CNF, CONFIG.PHA, CONFIG.SYS, CONFIG.CON) and during other working sessions will be called automatically as default settings.**

**In order to come back to a standard configuration provided with INFOREX just reload the STANDARD.CNF file.**

If you wish to work with other previous settings, load a corresponding ***.CNF file, which has been created earlier. *To load* previously arranged settings, get the *Settngs* window by the [***F6***] (***Load***) key, disable a current configuration file name (CONFIG) and enable the name of settings you are going to load from the file list. Then press the [***F6***] key to see if the loaded settings in the *Paths, Phases, Systems,* and *Containers* windows are those you need.

*Buffers window* is now inaccessible: the ability to change the list of oxygen buffers currently available in INFOREX-4.2 will be present in the forthcoming versions of the database.

### *4.2. General System Information (GSI)*

Press the [***F2***] key in the *Main Menu* and wait for a moment until two windows appear in the frame called *General System Information*.

*The left GSI window* is a passive informational one serving to display the number of master records currently available in the database (written in the CONDIT.EXP file - Fig. 3.2). These records are subdivided in accordance with the *Natural/Synthetic* or *Dry/Wet* system indicators, as well the *Presence/Absence* of volatiles, and run durations.

*The right GSI window* is an active one, incuding a list of filenames for experimental glasses and minerals currently available in the database and enabled during a working session (the numbers to right of the filenames inform how many records are present in the file considered - Fig. 6). These files can be browsed or printed out using the [***F5***] functional key.

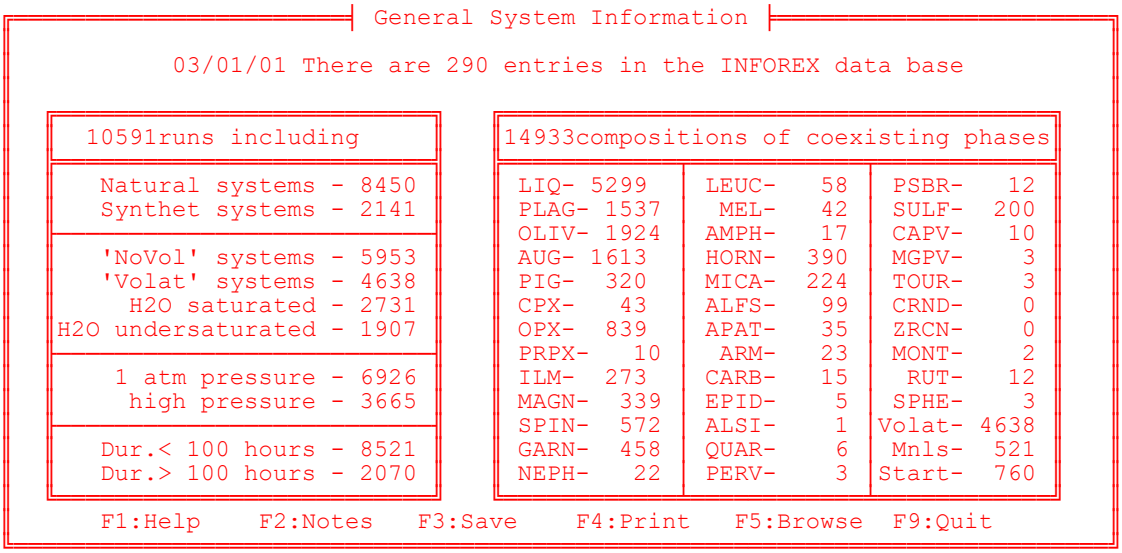
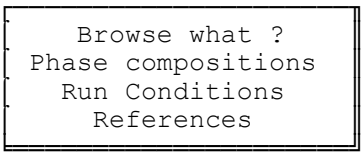



**Figure 6**. Screen image of the **General System Information** option
*This image can be saved as GENERAL.INF file or printed out using the F3 or F4 keys*

*Using the [**F5**] (**Browse**) function.*

This is an important informational option which allows one to understand how the INFOREX database is organized and to see at the monitor different types of records used to develop the informational system. After pressing the [***F5***] (***Browse***) key one can see a small menu asking for 3 kinds of information you can browse now:

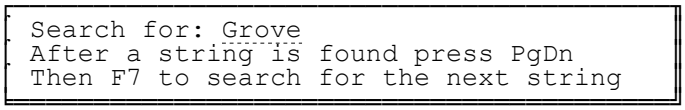



Use the [↑] or [↓] keys to select an informational object and press “Enter” to activate a special internal viewer which allows one to scroll a datafile (e.g., CONDIT.EXP), to print out a part of the viewed information or to conduct a search for a text symbol(s) in the file considered (*some other options are shown at the bottom of the viewer window*).

If you selected *Phase compositions,* the first name in the list of phase composition files will be highlighted, so that one can choose any file to browse navigating using the arrow keys and pressing “Enter”.

If you selected *Run Conditions* or *References,* you can browse the CONDIT.EXP and BIBL.TXT files. During scrolling the BIBL.TXT file one can search for the names of authors whose publications or unpublished experimental studies were included into INFOREX database, as well to search for any kind of specific petrological (geochemical, geographic, etc.) terms based on given keys words.

To initiate the searching option, press the [***F7***] key in the *Browse* mode and a prompt will appear:




To conduct a search, type a word of interest (e.g., *Grove*) and press “Enter”. If a string including the word will be found in the BIBL.TXT file, the in-built viewer will highlight the string(s) and stop the operation. To continue the searchig, one should press the [***PgDn***] key, followed by the [***Shift***]+[***F7***] combination, if you are going to search for the same symbols. Press the [***F7***] key to search for a new entry.

After completing the operations with the *Browse* option press “Esc” (*see prompt at the bottom*) to return to the *GSI windows*. Then press the [***F9***] key to quit the *GSI* option.

### *4.3. View / Edit / Input Data Files (V/E/I)*

As mentioned above, the basic unit of the database is an individual experimental study recorded in the BIBL.TXT file and linked with master records in the CONDIT.EXP file (Fig. 2). The *V/E/I* option of the Main Menu offers the user an ability to work with the main database units. Using this option one can scan the bibliography records page by page or select them at once.

#### *4.3.1. The use of View option*

After you pressed the [***F3***] key of the Main Menu you will see a frame including two windows (Fig. 7). The upper one is active and contains the first reference available in the INFOREX database, whereas the second one, called “*Experimental conditions and resultant phase assemblages*”, is passive inculding only empty fields below the title. One can use the [***PgUp***] and [***PgDn***] keys to scan the bibliography records page by page, followed with pressing “Enter” to select an experimental study.

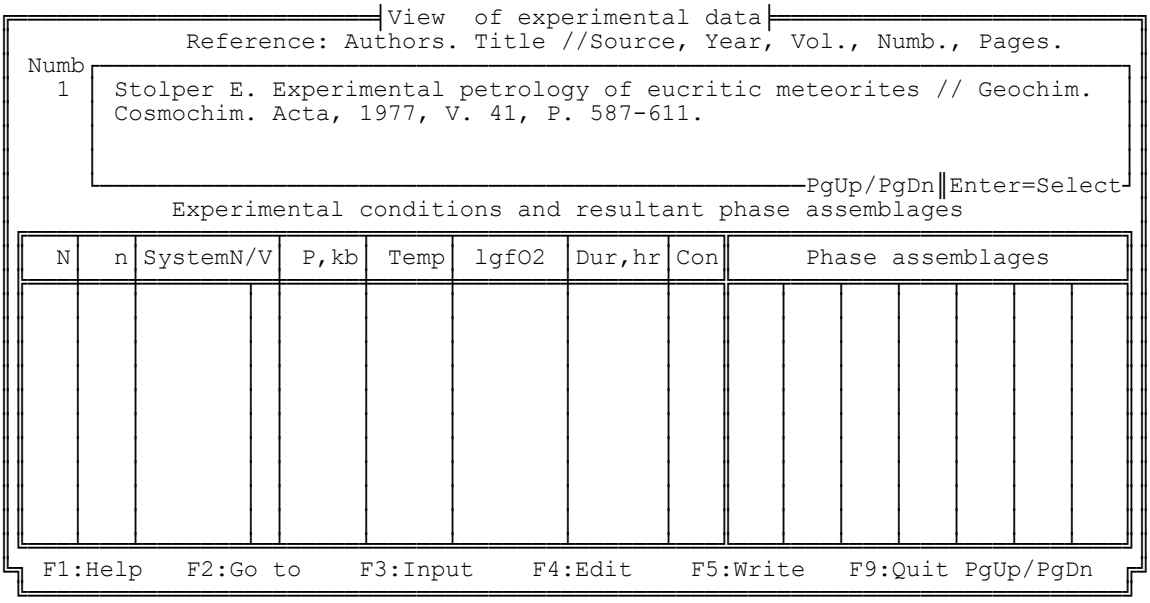
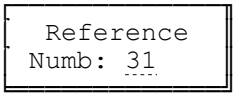



**Figure 7**. Screen image of the **View** option at an initial stage

If you need to quickly find out a reference based on its INFOREX number (which might be known, if you have browsed the BIBL.TXT file using the *General Information* option), just press the [***F2***] (***Go to***) key and type the number in a small window, e.g.




After few seconds of searching through the INFOREX database, the UI will display master records of the CONDIT.EXP file corresponding to a selected experimental study (Fig. 8).

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 resultant 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 | AF1 | | |
| | 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

**Figure 8**. Screen image of the **View** option after selecting a reference

Simultaneously, 2 functions from the initial frame will be changed: ***F2:Go to*** is transformed to ***F2:Notes***, and ***F3:Input*** is transformed to ***F3:Next***. Use the [***F3***] key to get compositional files concerned with the selected study: starting materials or phase composition records linked with the main master records will subsequently appeare on the screen. Calling for the last mineral composition file will automatically result in a sound and appearence of the string:

*No more phase compositions! Press any key to continue.*

One should then press any alphanumeric key either the [***F9***] key to return to the *Main Menu*, or [***Shift***]+[***F3***] to return to the upper "*Reference*" window.

Using the [***F5***] (***Write***) key, one can specify a file name to store different master and compositional records at any stage of the operations: this option was developed to allow the user to extract specific subsets of experimental information available in the study of interest. If you press the [***F5***] key a small window will appear:

```
Enter File name (or PRN)
N
```

where "*N*" is a system prompt: we suppose you are going to save these data as a file named "*N*" (where "*N*" corresponds to the INFOREX reference). Sure, one can overtype any appropriate name. To printout the information requested just type *PRN* and press "Enter".

### 4.3.2. *The use of Edit option*

Sometimes, the user may encounter an error in the database, e.g. during performing a search for mineral-melt compositional pairs (see *chapter 4.5*, BASE.ERR file), or errors due to misprints in the source papers. To correct the problems or to make changes in the selected study one should use the *Edit* option. To initiate the *Edit* option, press the [***F4***] (***Edit***) key at any stage of the use of the *View* option. A highlighted field will appear in the upper left part of the lower window: move the highlighted field to the field of interest with arrow and ***PgUp/PgDn*** keys and make all of the necessary changes, followed with pressing "Enter" after each correction (Fig. 9).

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.

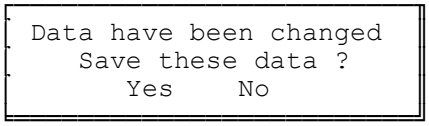
Contents of major components in LIQ - phase, wt.%

| 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 9**. Screen image of the **Edit** option after selecting a reference and scanning the LIQ.EXP compositional datafile

When you press the [***F3***] (***Next***) key in order to go to the next dataset availavle for the selected experimental study the system will ask if you want to save the corrected data:



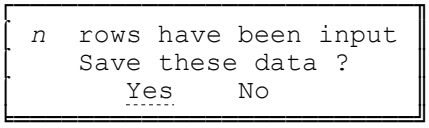

Your choice! Press the [***F9***] key to quit the operation.

**Note: as a rule, our team provides a ternary personal control of the experimental information to be input into the INFOREX database.**

*4.3.3. The use of Input option*

This option works as an in-built editor developed to introduce into INFOREX a new experimental information from the literature. In fact, its use is convinient only if you have a small batch of experimental data (*no more than 10-15 experiments with 10-20 phase compositions*), because the *Input* option does not allow one to save uncompleted datasets or to continue the loading at another time. This is the main reason why ***we recommend users to call for the EID-option to input new experimental data (see the chapter 4.6).*** Nevertheless, a detailed description of the *Input* option is presented below.

To initiate the *Input* option one should press the [***F3***] (***Input***) key in the initial *View* option frame (Fig. 7). After pressing the [***F3***] key, the UI gives the new number (*Last+1*) to the dataset to be entered and clears the input fields of the "*Reference*" window. A full blinking cursor appears therein: this means a new bibliography information is requested (at this stage the system is in overwrite mode, therefore the cursor responds only to the arrow keys). All other *Input* options are disabled now but the ***F3*** one called "*End of reference Input/Edit*": type the reference in any format (*no more 4 strings!*) and press the [***F3***] key. After that there will be a question if you want to save the new bibliography information:



Choose “Yes” by pressing “Enter”, if you are sure all is correct with your new reference. Same requests will appear in the screen when you are working with the master or compositional records.

**Note: the input fields are usually highlighted on the screen, therefore if you are going to input a number or a string that is shorter than the input field you shoud press the “Enter” key to finish the operation. If the string to be input is equal to the length of the highlighted field the input control system will automaticaly close the current operation followed with the movement to the next input field.**

After finishing the “*Reference*” operation the input highlighted field will be moved to a set of empty fields corresponding to those of master records in the CONDIT.EXP file. All of the fields are tabulated allowing one to type the run numbers, system indecies, pressures, and other experimental conditions (Fig. 10). The system automatically controls the number of units (“1”) presented after each phase indicator (Lq1, PL1, etc.), sending in the UI memory the number of empty strings which should be filled later in the phase composition datafiles.

Input of experimental data

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

Numb 102: Nielsen R.L. Experimental study of high temperature plagioclase-melt equilibria in high magnesium tholeiitic system (unpublished data, 1992).

Experimental conditions and resulted phase assemblages

| N | n | SystemN/V | | P,kb | Temp | lgfO2 | Dur,hr | Con | Phase assemblages | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 102 | 1 | BAS - | N | 0.0 | 1250 | QFM-1.0 | 72.0 | PTL | LQ1 | PL1 | OL | | | | |
| | 2 | BAS - | N | 0.0 | 1260 | QFM-1.0 | 60.0 | PTL | LQ1 | PL1 | OL | | | | |
| | 3 | BAS - | N | 0.0 | 1270 | QFM-1.0 | 60.0 | PTL | LQ1 | PL1 | OL | | | | |
| | 4 | BAS + | N | 0.0 | 1270 | QFM-1.0 | 60.0 | PTL | LQ1 | PL1 | | | | | |
| | 5 | BAS + | N | 0.0 | 1280 | QFM-1.0 | 48.0 | PTL | LQ1 | PL1 | | | | | |
| | 6 | BAS + | N | 0.0 | 1290 | QF | 0.0 | | | | | | | | |
| | 7 | - | | 0.0 | 0 | | 0.0 | | | | | | | | |
| | 8 | - | | 0.0 | 0 | | 0.0 | | | | | | | | |
| | 9 | - | | 0.0 | 0 | | 0.0 | | | | | | | | |
| | 10 | - | | 0.0 | 0 | | 0.0 | | | | | | | | |

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

**Figure 10**. Screen image of the **Input** option during work with main master records
*This is an example of 1992 where only 101 studies were included into the INFOREX database*

The *Input* control system identifies strings that have been ready for the automatic input by the first nonempty field in the phase assemblage codenames area for the run conditions master records, and by first 3 nonzero positions for the phase composition records (it means at least 3 first positions in each highlighted field should be filled in).
**Note: most of the *Input* fields are valid only for numbers or alphanumeric strings, and if you press an alphabetic key in the numeric field you will hear a beep and nothing appears on the screen. So, be sure you press permissable keys.**

**But some fields allow both alphanumeric string and numbers to be input, for example the "lgfO2" field of CONDIT.EXP file permits both a number like "-12.58" or a string like "QFM-1.2". If you mistakenly type the "number" -12.S8 instead of -12.58, this error will not be detected here by the *Input* control system and later the program will interprete the "number" -12.S8 as -12.00.**

In the case of large batches of experimental data (of about 50 experiments with hundreds of microprobe analyses) *there is an ability to load these data in two stages*. To do this one should first complete the fields of "*Phase Assemblages*" for all master records to be entered. Due to such a preliminary operation the *Input* control system "knows" how many strings need to be reserved for the input of chemical compositions in each of the phase composition files. So, now one can conduct an input of "uncompleted" datasets including major element contents, e.g. by filling in only the first three columns ($SiO_2$ contents) within the compositional strings, followed with saving these uncompleted datasets. Such a "template" can be completed later during a second stage of the input using the *Edit* option.

Press any alphanumeric key followed with either [***F9***] to return to the *Main Menu*, or [***Shift***]+[***F3***] to return to the "Reference" window.

**Note: Beginninig from the INFOREX-2.0 release the data input is rather easier due to a new ability to *Mark* and Copy the whole input string(s), if there are a few similar strings in your source data. This option is now available for the "*New reference input*" mode only.**

**To copy string(s) in the "*New reference input*" mode you should place the cursor at the first string to be copied (using the arrows and *PgUp/PgDn* keys) and press [*F4*] (*Mark*) key (*we assume that you have already pressed it once to initialize the Edit routine and you are seeing now the full-block cursor in your screen*). A blinking "*Mark*" label and bell indicate that this *Mark*-option is activated. Use arrows and *PgUp/PgDn* keys to highlight strings to copy and press [*F4*] key again to fix the highlighted block. Place the cursor before the string where you are going to insert the block and press [*F4*]: the block will be inserted before the string. Press [*Esc*] to cancel copying at any stage of the operation.**

*Again we emphasize, that our own experience in the practical work with the INFOREX database has shown that the use of Export/Import operations is much more preferable to input new experimental information.*

### *4.4. Selecting Run Conditions (SRC)*

This is one of the most important INFOREX functions oriented to the following 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:

- 5 general types of silicate systems investigated, such as ***Terrestrial***, ***Lunar***, ***Meteoritic***, ***Planetary*** (Venus, Martian, etc.), and ***Synthetic***
- names of igneous rocks (***BAS*** - basalts, ***KOM*** - komatiites, ***SYN*** - synthetic, etc. - see NOTES.TXT in *Appendix 1*)
- combinations of volatile components ($CO_2$, $H_2$, $H_2O$), including an ability to select fluid saturated and/or undersaturated experiments
- flags of the presence or absence of a direct chemical information on water contents and $Fe^{3+}/Fe^{2+}$ ratios in experimental glasses
- types of containers used in the experiments (***PTL*** - Pt loops, ***AGP*** - Ag-Pd capsules, etc. - see NOTES.TXT in *Appendix 1*)
- experimental conditions, including the range of temperatures, pressures, run durations, and oxygen fugacities)
- the range of major component contents or some routinely used petrochemical ratios for available experimental glasses (here is also a new ability to specify a set of glasses corresponding to igneous rock series based on the $SiO_2$ - $Na_2O+K_2O$ diagram).

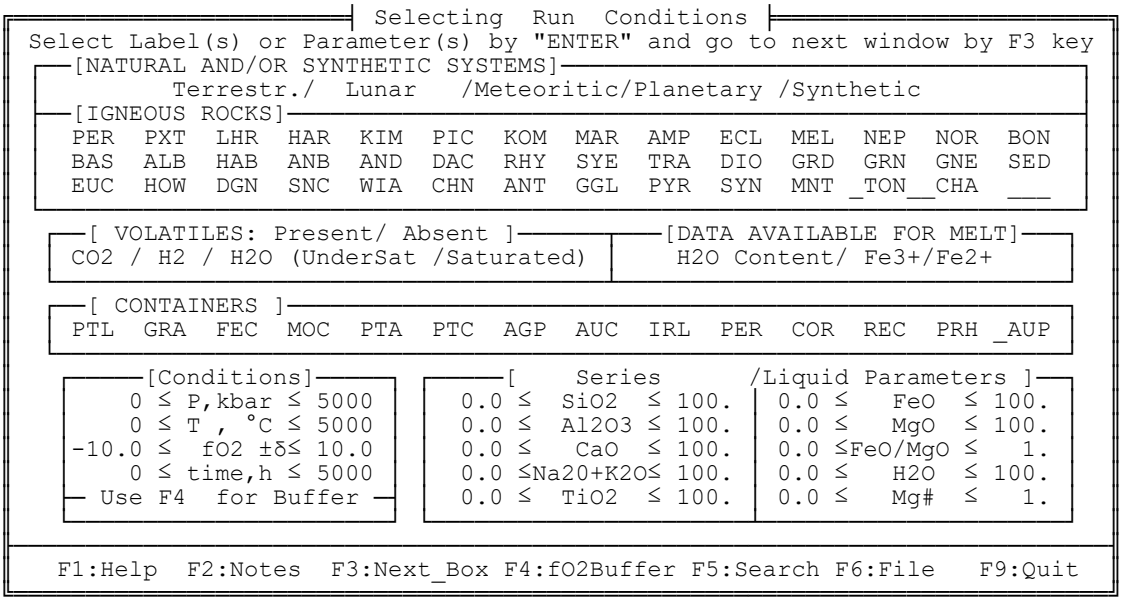



**Figure 11.** Screen image of the **Selecting Run Conditions** option

The screen display for presenting the *SRC* option is given in Figure 11. It contains a set of countered boxes: transition from one box to another is by means of pressing the [**F3**] (***Next_box***) key (the [***Shift***]+[***F3***] combination allows one to come

back to a previous box or window). To setup a parameter to filter data one should move the highlighted field to the parameter field and press “Enter” or type a number.

**Note: All items within the first 4 groups of the filters mentioned above are related to each another by logical “*OR*”, whereas logical “*AND*” is the relation between the main filter groups. Items of “Conditions” and “Series/Liquid Parameters” are related by logical “*AND*”, just like the groups itself. It means if you selected the runs with *Lunar* and *Meteoritic* materials you will find the CONDIT.EXP master records including both eucrites (*EUC*), SNC meteorites (*SNC*), lunar basalts (*BAS*), green glasses (*GGL*), and others. But if you have used an additional restriction, such as SNC in the “Igneous Rocks” window, you will find only experiments on SNC meteorites.**

*An attractive feature of the SRC option is the ability to specify the range of redox conditions of interest.* To perform this operation, one should specify a type of oxygen buffer and the range of oxygen fugacities with respect to the given buffer (*log units*). To give the buffer name, move the highlighted field to the “**fO2±δ**“ field in the “*Conditions*“ window and press the [***F4***] (***fO2 Buffer***) key. As a result a window will appear in the screen:

```
╔═[Esc=Exit]═══[Enter=Select]═╗
║ IW      | Myers,Eugster,1983 ║
║ WM      | Myers,Eugster,1983 ║
║ IM      | Huebner J.S.,1971  ║
║ MH      | Myers,Eugster,1983 ║
║ QFM     | Myers,Eugster,1983 ║
║ IQF     | Myers,Eugster,1983 ║
║ NNO     | Huebner J.S.,1971  ║
║ CCO     | Myers,Gunter,1979  ║
║ MMO     | Mn3O4     -MnO     ║
║ COC>5kb | Woermann et al.,1977 ║
║ COC<5kb | French B.H., 1966  ║
║ GRS     | Graphite-COH       ║
║ GCH     | Graphite-methane__ ║
║ ___     | RESERVED           ║
╚═══[Select buffer by ↓/↑ keys]═╝
```

Use the arrow keys to select a needed buffer by a highlighted field and press “Enter”: selected buffer name appears at the place of **fO2** label in the “*Conditions*” window.

*Searching throughout the database* can be started from any field in the screen: press the [***F5***] (***Search***) key and wait for a few seconds until the *Search* system informs you that 3 files, characterizing the experiments selected, are created in the D:\INFOREX\SAVE\.. directory:

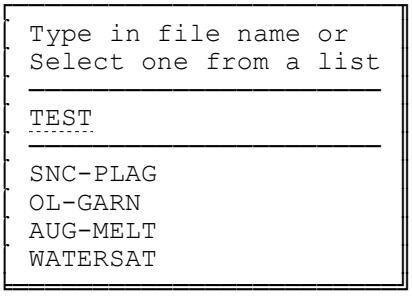
```
┌──────────────────────────────────────────────┐
│  Files data1_.inf, data2_.inf, and data3_.inf │
│        containing selected information       │
│   have been created.Press any key to continue │
└──────────────────────────────────────────────┘
```

These auxiliary files involve short references, a list of phase assemblages and master records for all individual runs satisfying the previously defined criteria. Those files (as well some others - see *Table 1*) serve as temporary data files for the following *SPA* procedure. If no data match your restrictions, another window will appear in the sceen with the mismatch information.

Beginning from the INFOREX-4.0 (1997) release, *the SRC option includes the ability to save configurations of the searching* to a separate file or load some previously saved configurations from the screen. For the purpose a special function "*File*" was developed. We recommend using this function first before calling for the *Search* procedure. During use of *Setting Phase Assemblages* option the INFOREX UI creates output files (e.g., including olivine-melt or spinel-garnet equilibria information - see below) which in the first string contain a file name of the "*Search*" configuration, as well a date of conduction the search. So, the function "*File*" allows one to find out a previously used "*Search*" configuration, if you have forgotten what kinds of filters and restrictions were used previously.

To save or to load a "*Search*" configuration, press the [***F6***] (***File***) key from any field in the *SRC* screen - a small menu will appear on the monitor:

Select any of the functions by the ***PgDn/PgUp*** keys and press "Enter". A place for writing the "*Search*" configuration, as well a list of previously saved setting will appear in a frame:




Type a new file name (e.g., *TEST*) if you are going to save (*Write*) a "*Search*" configuration, or select another one if you want to load (*Read*) previously saved settings. Each name written using the "*File*" function will be saved as *.SEL file (e.g., *TEST.SEL*) in the D:\INFOREX\SAVE\.. directory. Your choice !

*To perform a new search*, one should press the [***F9***] (***Quit***) key to return to the *Main Menu*, followed by pressing the [***F4***] key to call for the *SRC* option again.

### *4.5. Setting Phase Assemblages (SPA)*

This option is designed for the purpose of creating phase equilibria compositional files which could be used in further thermodynamic processing and analysis of experimental information. *It works only if the SRC option has created a set of auxiliary files satisfying some previously defined criteria (Table 1)*.

Three windows appear on the screen when one calls the *SPA* option from the *Main Menu* by pressing the [***F5***] functional key. In the first, all phase assemblages are listed that have appeared in the data subset search-matched in the *SRC* procedure, whereas the second contains a list of shortcut references to experimental investigations where these data were described (Fig. 12).

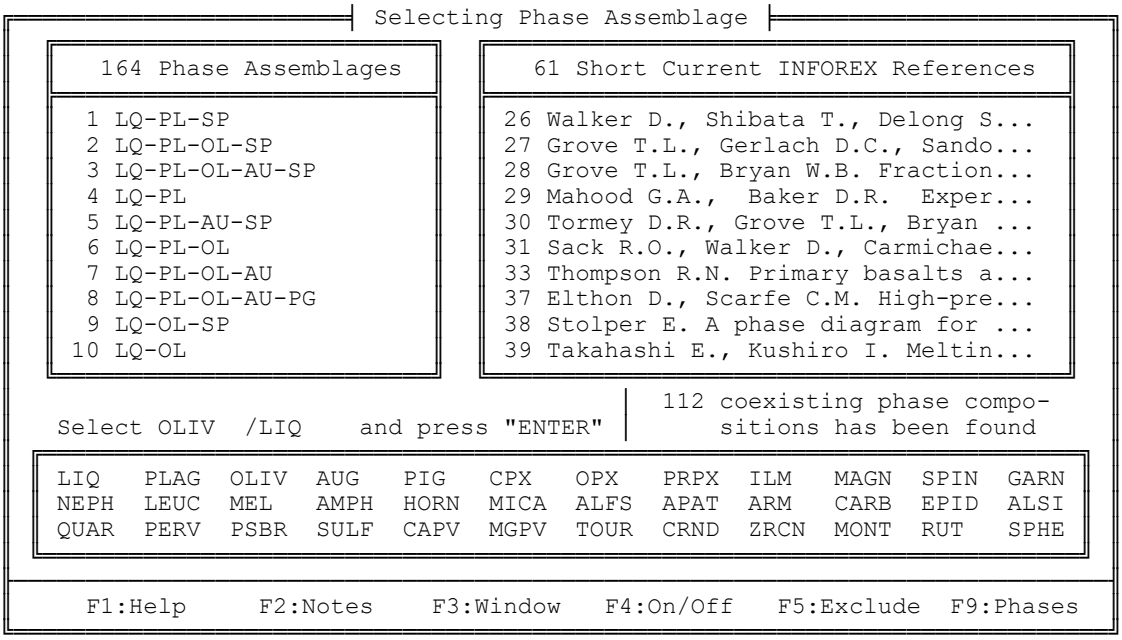



**Figure 12.** Screen image of the **Setting Phase Assemblages** option (*after selecting Olivine-Melt equilibrium*)

Using the [***F3***] (***Window***) key one can switch between these upper two windows. Pressing the [***F4***] (***On/Off***) key followed with the [***F5***] (***Exclude***) key allows one to exclude from these lists any phase association or an entire experimental investigation. This is convenient especially if only a single multiphase assemblage is required, such

as locating the compositions of melts equilibrated with olivine, plagioclase, pyroxenes, and spinel.

**Note: The *On/Off* function sets the disabling flag "√" in front of a selected phase assemblage or a shortcut reference: all strings marked to disable can be excluded from further processing by the *Exclude* function. *Important*: none of the erased strings can be enabled with the *SPA* option again! One should repeate a previous *SRC* session to correct a disabled mistake if necessary.**

When the desired arrangement is completed, the user can proceed to the third window containing the full list of phases (experimental products). It can be done by pressing the [***F9***] (***Phases***) key - a small menu appears on the screen:

```
Mineral-Melt Equilibria
Two mineral Equilibria
Only melt compositions
```

Significance of these functions with some practical examples will be given in the following paragraph.

*If you have selected "Mineral-Melt Equilibria"* or "*Only melt compositions*" (followed by the "*Melts Equilibrated with a Given Mineral*" function) the *SPA* option allows the user to select one of the mineral phases in the third window (assumed that liquid is to be the second coexisting phase). A highlighted field appearing at the first name field should be moved by the arrow keys to the name of interest. Press "Enter" and in a few seconds the number of mineral-melt coexisting pairs extracted will be displayed on the screen (Fig.12); simultaneously a prompt will appear:

```
Press any key to continue...
```

Press "Enter" and a message will inform you that a corresponding file has been created and stored in the D:\INFOREX\SAVE.. directory. For example, if at this stage you selected OPX this message will look like:

```
File OP_LQ.DAT containing phase compositions
has been created. Press any key to return to main menu
```

*If the "Two mineral equilibria" function has been selected*, move the highlighted field to the name of first phase requested and press "Enter", then do the same for the second phase. The system prompts will look like those described above.

*If you have selected "Only melt compositions"* (followed by the "*Melts Equilibrated with All Phases*" or "*Melts To test Fe3+/Fe2+ Ratio*" functions) the *SPA* procedure will also show how many liquid compositions were found and a corresponding file (see below) created.

```
OP_LQ.SEL (03/21/96 16:50:12)
 77|   2|SNCM- 2|N|   0.0|  1270|   -7.70|   49.0|PTL|LQ1|OL1|OP1|SP |   |   |
166|   1|CHNM- 1|N|   0.0|  1350|  -11.20|   72.0|PRH|LQ1|OL1|OP1|   |   |   |
166|   2|CHNM- 1|N|   0.0|  1328|  -11.43|   92.0|PRH|LQ1|OL1|OP1|   |   |   |
166|   5|CHNM- 1|N|   0.0|  1300|  -11.73|  122.0|PRH|LQ1|OL1|OP1|   |   |   |
166|   6|CHNM- 1|N|   0.0|  1300|  -11.73|   67.0|PRH|LQ1|OL1|OP1|   |   |   |
166|   7|CHNM- 1|N|   0.0|  1275|  -12.01|   97.0|PRH|LQ1|OL1|OP1|   |   |   |
166|   8|CHNM- 1|N|   0.0|  1220|  -12.66|  120.0|PRH|LQ1|OL1|OP1|   |   |   |
166|   9|CHNM- 1|N|   0.0|  1200|  -12.90|  120.0|PRH|LQ1|OL1|OP1|   |   |   |
166|  10|CHNM- 1|N|   0.0|  1180|  -13.16|  120.0|PRH|LQ1|OL1|OP1|   |   |   |
166|  11|CHNM- 1|N|   0.0|  1170|  -13.32|  168.0|PRH|LQ1|OL1|OP1|   |   |   |
166|  12|CHNM- 1|N|   0.0|  1170|  -13.32|  114.0|PRH|LQ1|OL1|OP1|   |   |   |
166|  17|CHNM- 2|N|   0.0|  1220|  -12.66|   48.0|PRH|LQ1|OL1|OP1|   |   |   |
166|  18|CHNM- 2|N|   0.0|  1200|  -12.90|  120.0|PRH|LQ1|OL1|OP1|   |   |   |
166|  20|CHNM- 2|N|   0.0|  1170|  -13.32|  168.0|PRH|LQ1|OL1|OP1|   |   |   |
OPX.EXP
 55.74   .08   .50 12.62   .37 29.88  1.24   .02   .00   .00   .40   .00  77  2
 55.70  0.00  0.29 14.20  0.28 28.90  0.40  0.00  0.00  0.00  0.61  0.00 166  1
 55.00  0.00  0.37 15.80  0.30 27.60  0.54  0.00  0.00  0.00  0.71  0.00 166  2
 55.30  0.00  0.41 16.40  0.29 27.60  0.61  0.00  0.00  0.00  0.72  0.00 166  5
 55.10  0.00  0.43 16.80  0.31 27.30  0.61  0.00  0.00  0.00  0.70  0.00 166  6
 55.10  0.00  0.48 17.40  0.33 27.40  0.78  0.00  0.00  0.00  0.79  0.00 166  7
 54.30  0.00  0.66 18.20  0.35 25.50  1.38  0.00  0.00  0.00  0.69  0.00 166  8
 54.40  0.00  0.47 17.40  0.36 25.60  1.82  0.00  0.00  0.00  0.43  0.00 166  9
 54.20  0.00  0.44 17.80  0.37 24.60  2.44  0.00  0.00  0.00  0.49  0.00 166 10
 54.10  0.00  0.42 18.00  0.39 24.10  2.86  0.00  0.00  0.00  0.50  0.00 166 11
 54.50  0.00  0.60 17.00  0.40 25.70  1.84  0.00  0.00  0.00  0.45  0.00 166 12
 53.40  0.00  0.70 20.60  0.27 24.00  0.90  0.00  0.00  0.00  0.17  0.00 166 17
 53.30  0.00  1.17 20.80  0.29 22.80  1.42  0.00  0.00  0.00  0.83  0.00 166 18
 52.40  0.00  1.09 20.90  0.31 22.10  2.12  0.00  0.00  0.00  0.72  0.00 166 20
LIQ.EXP
 50.47   .98  7.98 17.38   .56 10.98  9.52   .70   .00   .00   .27   .00  77  2
 52.10  0.23  5.64 23.30  0.44 14.60  4.52  0.01  0.00  0.00  0.74  0.00 166  1
 50.90  0.26  6.48 23.20  0.42 12.90  5.12  0.02  0.00  0.00  0.77  0.00 166  2
 50.60  0.29  7.21 24.30  0.40 12.10  5.69  0.01  0.00  0.00  0.77  0.00 166  5
 50.80  0.28  6.95 24.50  0.41 11.80  5.50  0.03  0.00  0.06  0.70  0.00 166  6
 50.60  0.38  8.50 23.40  0.41 10.40  6.85  0.03  0.00  0.07  0.72  0.00 166  7
 48.90  0.44 11.90 21.20  0.35  8.54  8.59  0.03  0.00  0.40  0.44  0.00 166  8
 50.70  0.47 13.00 17.80  0.32  7.31  8.39  0.69  0.00  0.52  0.38  0.00 166  9
 53.80  0.44 13.50 16.00  0.27  6.13  8.16  1.29  0.00  0.16  0.27  0.00 166 10
 49.60  0.50 14.80 16.80  0.30  6.70 10.10  0.12  0.00  0.14  0.29  0.00 166 11
 54.20  0.45 14.00 15.00  0.27  5.80  8.00  1.58  0.00  0.36  0.22  0.00 166 12
 49.10  0.35  9.47 24.60  0.30  7.97  7.84  0.05  0.00  0.20  0.43  0.00 166 17
 50.80  0.40 11.10 22.00  0.29  6.85  8.11  0.33  0.00  0.14  0.43  0.00 166 18
 52.90  0.42 12.10 18.60  0.24  5.79  8.64  1.01  0.00  0.19  0.27  0.00 166 20
```

**Figure 13**. An example of OP_LQ.DAT file used to develop *Opx*-melt geothermometers for meteoritic igneous systems (Ariskin et al., 1997*b*) created using the "*Mineral-Melt Equilibria*" function

***Significance of the main "Phases" functions***

Use the arrow keys followed by pressing "Enter" to select one of the 3 functions:

(1) "*Mineral-Melt Equilibria*" provides an ability to find out an experimental information on the equilibrium of a given mineral with melts (glasses), e.g. *orthopyroxene-melt* or *spinel-melt*. Files like ****_LQ.DAT** (*OP_LQ.DAT* or *SP_LQ.DAT*) will be created by the function and stored at the D:\INFOREX\SAVE.. directory (Fig.13).

(2) selecting "*Two mineral equilibria*" means you are going to request information on a two solid phases equilibrium, e.g. *olivine-garnet* ot *augite-orthopyroxene*. Files like ****_**.DAT** (*OL_GR.DAT* or *AU_OP.DAT*) will be created by the function and stored at the D:\INFOREX\SAVE.. directory:

```
OL_SP.SEL (05/14/97 12:50:37)
158|   3|PERS- 1|N|  10.0|  1360|      ND|   58.0|GRA|LQ1|OL1|OP1|SP1|   |   |
158|   4|PERS- 1|N|  10.0|  1350|      ND|   53.7|GRA|LQ1|OL1|OP1|SP1|   |   |
158|   8|PERS- 1|N|  10.0|  1330|      ND|   71.9|GRA|LQ1|OL1|OP1|AU1|SP1|   |
158|  14|PERS- 1|N|  10.0|  1300|      ND|   72.0|GRA|LQ1|OL1|OP1|AU1|SP1|   |
158|  16|PERS- 1|N|  10.0|  1280|      ND|   51.6|GRA|LQ1|OL1|OP1|AU1|SP1|   |
158|  18|PERS- 1|N|  10.0|  1270|      ND|   97.9|GRA|LQ1|OL1|OP1|AU1|SP1|   |
158|  19|PERS- 1|N|  10.0|  1270|      ND|  151.3|GRA|LQ1|OL1|OP1|AU1|SP1|   |
175|  48|PERS+ 0|N|  15.0|  1320|      ND|   48.0|GRA|LQ1|OL1|OP1|AU1|SP1|   |
175|  53|PERS+ 0|N|  15.0|  1335|      ND|   48.0|GRA|LQ1|OL1|OP1|SP1|   |   |
OLIV.EXP
 40.70  0.00  0.06  8.44  0.09 51.10  0.30  0.00  0.00  0.00  0.29  0.00 158  3
 40.40  0.00  0.05  8.50  0.11 50.80  0.32  0.00  0.00  0.00  0.25  0.00 158  4
 40.50  0.00  0.07  8.60  0.10 50.50  0.34  0.00  0.00  0.00  0.24  0.00 158  8
 40.80  0.00  0.06  9.10  0.14 51.00  0.28  0.00  0.00  0.00  0.14  0.00 158 14
 40.80  0.00  0.03  8.98  0.13 49.80  0.22  0.00  0.00  0.00  0.13  0.00 158 16
 40.20  0.00  0.04  9.20  0.16 50.40  0.25  0.00  0.00  0.00  0.12  0.00 158 18
 40.70  0.00  0.00  9.14  0.11 50.50  0.22  0.00  0.00  0.00  0.13  0.00 158 19
 38.60  0.00  0.08 20.60  0.34 40.30  0.32  0.00  0.00  0.00  0.31  0.00 175 48
 39.00  0.00  0.11 21.90  0.37 38.70  0.33  0.00  0.00  0.00  0.15  0.00 175 53
SPIN.EXP
  0.24  0.10 24.00 10.22  0.19 18.00  0.11  0.00  0.00  0.00 47.60  0.00 158  3
  0.23  0.14 24.50 10.90  0.14 18.00  0.15  0.00  0.00  0.00 46.80  0.00 158  4
  0.32  0.17 28.50  9.90  0.17 18.16  0.07  0.00  0.00  0.00 42.10  0.00 158  8
  0.05  0.09 37.60 10.00  0.12 19.78  0.09  0.00  0.00  0.00 32.90  0.00 158 14
  0.18  0.17 44.20  9.30  0.11 20.00  0.08  0.00  0.00  0.00 25.00  0.00 158 16
  0.19  0.09 44.20  9.50  0.11 20.40  0.05  0.00  0.00  0.00 25.60  0.00 158 18
  0.27  0.14 43.40  9.80  0.09 20.20  0.09  0.00  0.00  0.00 27.00  0.00 158 19
  0.48  0.66 27.60 22.40  0.31 11.80  0.00  0.00  0.00  0.00 36.70  0.00 175 48
  0.49  0.57 26.60 23.10  0.36 11.40  0.11  0.00  0.00  0.00 36.60  0.00 175 53
```

**Figure 14**. Example of OL_SP.DAT file characterizing *Olivine-Spinel* equilibrium created using the "*Two mineral equilibria* " function for the experiments conducted at 10-15 kbar on *Dry Synthetic* low-alkaline systems (run duration ≥ 48 hours)

(3) selecting "*Only melt compositions*" permits one to extract only experimental glass compositions, which can correspond to one of 3 additional restrictions:

```
┌──────────────────────────────────────┐
│ Melts Equilibrated with All Phases   │
│ Melts Equilibrated with a Given Mineral │
│ Melts To test Fe3+/Fe2+ Ratio        │
```

(3*a*) "*Melts Equilibrated with All Phases"* allows one to retrieve all experimental glass compositions, satisfying previously defined criteria: **LQ_LQ.DAT** file will be created here. This function is especially useful if one is interested in melt compositions representing a given set of phase assemblages, specified earlier in the upper left window (Fig. 12) using the [***F4***] (***On/Off***) and [***F5***] (***Exclude***) keys.

One can readily create a file including all glass compositions corresponding to a multiphase equilibrium, e.g. *Olivine-Orthopyroxene-Augite-Spinel-Melt*. Such an information might be used in further projectings of the liquid compositions onto ternary diagrams (see *chapter 4.7.5*), or for calibrations of equations describing liquidus temperatures of the mineral assemblage in terms of the liquid composition (*Longhi, 1991; Ariskin et al., 1997a*). An example of such a file is given in Fig. 15.

```
LQ_LQ.SEL (05/14/97 14:01:35)
 35|  43|LHR - 1|N|  30.0|  1550|      ND|   17.0|GRA|LQ1|OL1|AU1|OP1|GR1|    |
156|   1|LHR - 1|N|  45.0|  1650|      ND|    6.0|GRA|LQ1|OL1|OP1|AU1|GR1|    |
183|  27|LHR - 1|N|  30.0|  1470|      ND|   11.1|GRA|LQ1|OL |OP |AU |GR |    |
183|  28|LHR - 1|N|  30.0|  1460|      ND|   10.0|GRA|LQ1|OL |OP |AU |GR |    |
LIQ.EXP
 46.90  0.90 11.00  7.80  0.20 19.20 12.20  1.20  0.00  0.00  0.40  0.00  35 43
 45.90  0.00  9.70 10.40  0.00 19.00 10.40  0.70  0.00  0.00  0.50  0.00 156  1
 45.63  2.00 12.54 11.20   .19 15.24  8.98  2.06  1.88   .00   .28   .00 183 27
 46.73  2.23 13.09 10.14   .13 12.35  7.74  2.55  4.91   .00   .13   .00 183 28
```

**Figure 15**. Example of LQ_LQ.DAT file characterizing a high-pressure *Olivine-Orthopyroxene-Augite-Garnet-Melt* cotectics
created using "*Only melt compositions*" function coupled with "*Melts Equilibrated with All Phases"* for the experiments conducted on *Dry Terrestrial Harzburgites* at 30-45 kbar (run duration ≥ 4 hours)

(3*b*) "*Melts Equilibrated with a Given Mineral*" allows one to get experimental glass compositions being in equilibrium with a given mineral, independent of the type of phase assemblages or the presence/absence of microprobe information on the solid phase compositions. Files like ****_LQ.DAT** will be created by the function and stored at the D:\INFOREX\SAVE.. directory.

*For example*, one can readily create a file including all glass compositions in equilibrium with hornblende (*HB_LQ.DAT*), even if for part of the data the hornblende

compositions are unknown. Such an information might be used in further projectings of the liquid compositions onto ternary diagrams (see *chapter 4.7.5*).

Fig. 16 provides an example of such a file characterizing water-saturated melts equlibrated with hornblende (*Ariskin et al., 1997a*).

```
HB_LQ.SEL (05/14/97 14:41:19)
111|  36|BAS + 2|F|   2.0|   800|  -14.18|  102.0|AUC|LQ1|PL1|SF1|HB |OP |   |   |
111|  66|BAS + 2|F|   2.0|  1000|   -6.42|  144.0|AUC|LQ1|PL |AH |MT |CP |HB |OL |
112|  11|BAS - 1|F|   3.0|   850|      ND|  115.0|AUC|LQ1|PL2|HB1|   |   |   |
112|  12|BAS - 1|F|   3.0|   875|      ND|  137.0|AUC|LQ1|PL2|HB1|   |   |   |
112|  27|BAS - 2|F|   3.0|   850|      ND|  115.0|AUC|LQ1|PL2|HB1|   |   |   |
112|  28|BAS - 2|F|   3.0|   875|      ND|  137.0|AUC|LQ1|PL2|HB1|   |   |   |
112|  46|BAS - 3|F|   3.0|   850|      ND|  115.0|AUC|LQ1|PL2|HB1|   |   |   |
112|  47|BAS - 3|F|   3.0|   875|      ND|  137.0|AUC|LQ1|PL2|HB1|   |   |   |
112|  79|BAS - 5|F|   3.0|   850|      ND|  137.0|AUC|LQ1|PL2|HB1|   |   |   |
133|   3|BAS - 1|F|   5.0|   750|     QFM|  120.0|AGP|LQ1|PL1|MT |IL |HB1|*  |   |
133|  28|BAS - 2|F|   4.9|   725|     QFM|  216.0|AGP|LQ1|OL |PL1|IL1|HB1|SH1|PB1|
133|  42|BAS - 2|F|   4.9|   725|      MH|  216.0|AGP|LQ1|PL1|IL |HB1|PB |SH1|MI |
229|  12|BAS + 0|F|   2.0|   940|     QFM|  168.0|AGP|LQ1|AU?|HB1|*  |   |   |   |
LIQ.EXP
 67.04  0.11 14.40  1.32  0.03  0.42  1.35  5.14  3.09  0.00  0.00  5.95 111 36
 53.54  0.56 19.31  2.50  0.20  0.81  6.90  3.89  0.96  0.00  0.00  5.96 111 66
 74.37  0.36 16.15  1.76  0.09  0.25  3.25  2.70  1.01  0.09  0.00  0.00 112 11
 71.85  0.38 16.95  1.95  0.15  0.56  3.99  3.10  0.89  0.18  0.00  0.00 112 12
 74.13  0.43 17.06  1.68  0.10  0.24  2.38  3.77  0.12  0.13  0.00  0.00 112 27
 70.16  0.42 18.77  1.72  0.11  0.28  3.55  4.71  0.10  0.21  0.00  0.00 112 28
 74.29  0.35 16.20  1.89  0.11  0.43  3.52  2.57  0.54  0.12  0.00  0.00 112 46
 71.63  0.37 17.26  1.87  0.15  0.49  4.07  3.54  0.43  0.21  0.00  0.00 112 47
 72.68  0.31 17.05  1.52  0.10  0.12  2.91  3.59  1.56  0.19  0.00  0.00 112 79
 74.40  0.10 16.00  1.43  0.00  0.00  2.54  3.70  1.80  0.00  0.00  0.00 133  3
 75.80  0.10 15.80  1.06  0.00  0.00  2.44  2.40  2.40  0.01  0.00  0.00 133 28
 76.00  0.05 15.30  1.07  0.00  0.04  2.58  2.60  2.40  0.01  0.00  0.00 133 42
 60.29  1.46 21.44  2.60  0.17  0.29  6.71  5.02  2.02  0.00  0.00  0.00 229 12
```

**Figure 16**. Example of HB_LQ.DAT file characterizing *Hornblende-Melt* equilibrium created using "*Only melt compositions*" function coupled with "*Melts Equilibrated with a Given Mineral*" for the experiments conducted on *Water-saturated Terrestrial Basalts* at 2-5 kbar (run duration ≥ 100 hours)

(3*c*) selecting "*Melts To test Fe3+/Fe2+ Ratio*" function makes it possible to retrieve information, including experimental conditions, glass compositions and $Fe^{3+}/Fe^{2+}$ ratios in the glasses, if available.

File called **RE_LQ.DAT** will be created by the function and stored at the D:\INFOREX\SAVE.. directory.

```
RE_LQ.SEL (05/14/97 13:23:39)
152|   1|BAS - 0|N|   0.0|  1461|   -7.17|    5.0|PTL|LQ1|RE |   |   |   |   |
152|   3|BAS - 0|N|   0.0|  1459|   -8.21|    5.0|PTL|LQ1|RE |   |   |   |   |
152|   4|BAS - 0|N|   0.0|  1459|   -8.21|    5.0|PTL|LQ1|RE |   |   |   |   |
```

```
152|   6|BAS - 0|N|   0.0|  1459|   -9.21|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  11|BAS - 0|N|   0.0|  1459|   -6.15|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  12|BAS - 0|N|   0.0|  1459|   -6.15|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  20|BAS - 0|N|   0.0|  1362|   -7.93|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  35|BAS - 0|N|   0.0|  1366|   -8.91|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  38|BAS - 0|N|   0.0|  1366|   -8.91|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  50|BAS - 0|N|   0.0|  1363|   -6.81|    5.0|PTL|LQ1|RE|  |  |  |  |  |
152|  51|BAS - 0|N|   0.0|  1363|   -6.81|    5.0|PTL|LQ1|RE|  |  |  |  |  |
REDOX.EXP
152|   1|  10.34|   1.09|    .095|   .00|   .00|    .000| Fe2O3=1.111(FeOt-FeO)
152|   3|   8.79|    .76|    .078|   .00|   .00|    .000|
152|   4|  10.00|    .78|    .070|   .00|   .00|    .000|
152|   6|   8.81|    .58|    .059|   .00|   .00|    .000|
152|  11|   9.47|   2.04|    .194|   .00|   .00|    .000|
152|  12|   9.09|   1.58|    .156|   .00|   .00|    .000|
152|  20|   9.68|   1.10|    .102|   .00|   .00|    .000|
152|  35|  10.08|    .69|    .062|   .00|   .00|    .000|
152|  38|  10.49|    .57|    .049|   .00|   .00|    .000|
152|  50|   9.84|   2.07|    .189|   .00|   .00|    .000|
152|  51|   9.54|   1.96|    .185|   .00|   .00|    .000|
LIQ.EXP
 51.36  1.90 14.02 11.32  0.25  6.93 10.50  2.29  0.72  0.20  0.02  0.00 152  1
 52.57  1.94 14.23  9.47  0.25  7.03 10.70  2.38  1.08  0.13  0.02  0.00 152  3
 51.76  1.95 14.16 10.70  0.24  7.06 10.53  2.26  0.84  0.15  0.02  0.00 152  4
 52.03  1.95 14.23  9.33  0.25  7.04 10.77  2.06  1.64  0.14  0.02  0.00 152  6
 51.28  1.91 13.99 11.31  0.25  6.93 10.35  2.77  0.66  0.16  0.02  0.00 152 11
 49.97  2.86 14.04 10.51  0.19  7.17 10.89  2.74  1.20  0.25  0.04  0.00 152 12
 51.11  1.95 14.09 10.67  0.11  6.94 10.53  3.11  0.94  0.35  0.04  0.00 152 20
 51.93  1.97 14.41 10.70  0.10  6.88 10.87  1.72  0.68  0.56  0.03  0.00 152 35
 51.41  3.29 13.64 11.00  0.19  6.46  9.86  2.09  0.83  0.43  0.10  0.00 152 38
 52.39  1.96 13.96 11.70  0.22  7.06 11.17  2.38  0.20  0.17  0.03  0.00 152 50
 52.35  1.98 14.25 11.30  0.21  7.11 11.31  2.33  0.17  0.21  0.02  0.00 152 51
```

**Figure 17**. Example of RE_LQ.DAT file including information on $Fe^{3+}/Fe^{2+}$ ratios created using "*Only melt compositions*" function coupled with "*Melts To test Fe3+/Fe2+ Ratio*" for the experiments conducted on *Dry Terrestrial Tholeiite-Basaltic* systems at 1 atm, 1350-1500ºC, and oxygen fugacities ≤ *WM*

*Correction of mismatch problems*

Occasionally data mismatches may occur in the INFOREX database (usually, if a phase composition is absent whereas the flag of its presence "1" is present in the initial CONDIT.EXP file master record). If such a mismatch is recognized by the ***SPA*** option, the warning message will alert you of the problem:

```
 ATTENTION! A mismatch in INFOREX database encountered.
        See 'base.err' file to correct the problem.
```

*There are two ways to solve the problem*:

(1) contact Alexei Ariskin or Sergei Meshalkin at the address given above - we will correct all of the necessary INFOREX files and send the corrected files to the user;

(2) correct the database files independently, using the *Main Menu* options and information available in the BASE.ERR file (see *chapter 5.2*).

### *4.6. 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 to a separate file, whereas the second permits a complete dataset to be included in the INFOREX database. The exported file will appear in the D:\INFOREX\EXCHANGE\.. subdirectory and the file prepared for import must be in the same place and have "**.IMP**" extension.

So, if you need to conduct the *Exchange INFOREX Data* operations, press the [***F6***] key to choose the *EID* option from the *Main Menu* - a message will appear on the screen:

```
WARNING! Data import causes all previously created *.BAK files
   to be deleted. To save the files, leave the window now!
              Press any key to continue...
```

This is a warning against entering the *.BAK files created during a previous "*Import*" operation. Press "ESC " or "Enter" and you will find yourself in the window as shown in Fig. 18.

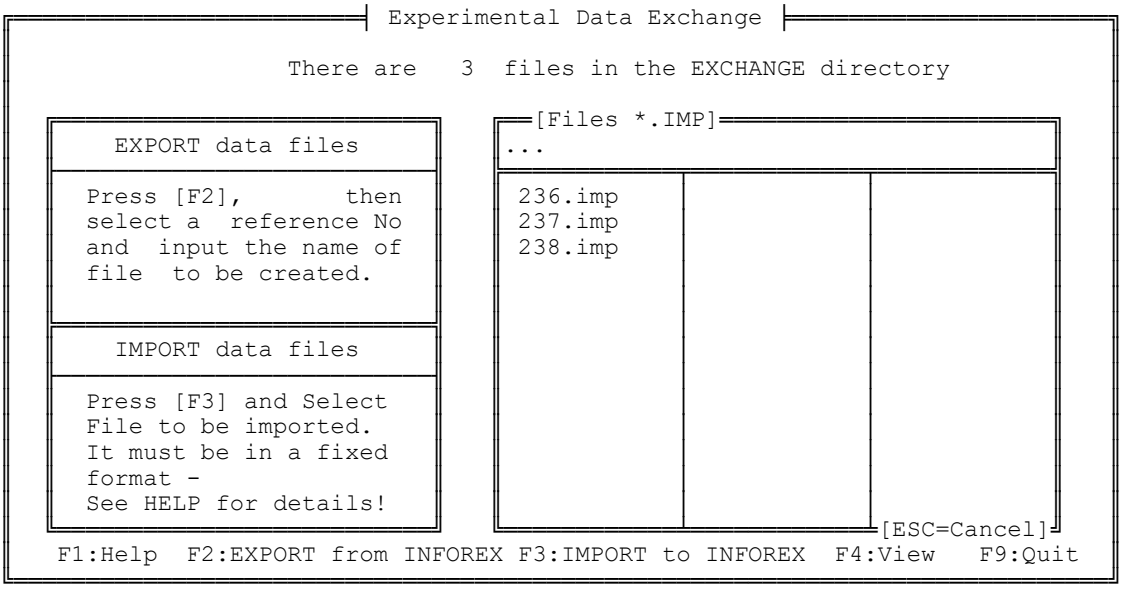



**Figure 18**. Screen image of the **Exchange INFOREX Data** option

*Export operations*

When you press the [***F2***] (***EXPORT*** *from INFOREX*) key a window appears on the screen like that provided with the *View* option (Fig. 7). Here one can choose an experimental work to save to a file: do this same way as in the *View of Experimental Data* window, using the ***PgUp/PgDn*** keys or "***Go to*** *(Reference)*" function. Press "Enter" to select a study and type a file name to be saved (up to 8 symbols) in the D:\INFOREX\EXCHANGE\.. subdirectory.

*Import operations*

When you press the [***F3***] (***IMPORT*** *to INFOREX*) key, a highlighted field will appear in the list of files to be imported, if there is at least one file having the ".IMP" extension (the number of such ****.IMP*** files available in the D:\INFOREX\EXCHANGE\.. subdirectory is displayed - Fig. 18). Using the arrow or ***PgUp/PgDn*** keys move the highlighted field to a file to import and press "Enter". The *EID* control system will check out if all is well with your imported dataset and in a few seconds a message might appear on the screen:

```
O'K with your import data.
  Press F5 to ACCEPT them
    or  ESC  to  CANSEL
```

In such a case press the [***F5***] key and your data will be properly inserted into the INFOREX database. If The *EID* control system encounters a problem in the initial datafile, a message will appear on the screen indicating what kind of errors should be corrected by the user in the file to be imported.

**Note: any file prepared for import should have the same format as files created during *Export* operations.**

**The following fields must be present in the records of the input file: number of the reference (the last number in your databaseincreased by 1) in the first string, up to four strings no longer than 71 positions - for bibliography, then word "CONDIT" followed by master records in the CONDIT.EXP file format (see Fig. 3). If this study has data on starting compositions, type word "START" in the next string followed by compositional master records. The next strings represent nonstandard file data (if any) in the formats of VOLAT.EXP, MNLS.EXP, SULF.EXP, and REDOX.EXP files preceded by corresponding headings - VOLAT, MNLS, SULF, REDOX. Finally, strings of glasses and mineral compositions appear with their headings. The format of all these strings must be exactly the same as in the corresponding files of the database.**

### *4.7. Perological Calculations (PC)*

Although we did not design the INFOREX system to be used as a comprehensive compilation of techniques for the thermodynamic processing of experimental data, a set of additional programs has been included into the system for use in petrological studies. Most of the programs were written in FORTRAN and include the development of mineral-melt equilibria equations (geothermometers), calculations of $Fe^{3+}/Fe^{2+}$ ratio and water solubility in experimental glasses, different major-element reformulations as well as calculations of normalization parameters for projecting glass compositions onto ternary diagrams (Fig. 19).

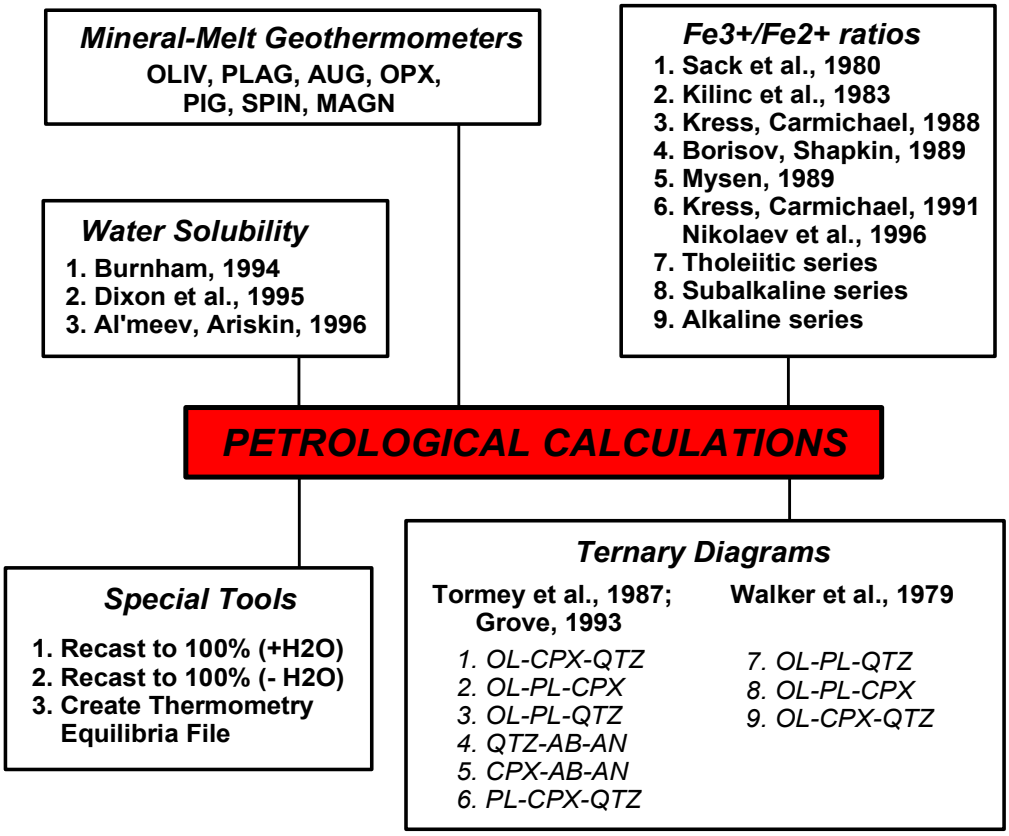



**Figure 19**. Main functions of the ***Petrological Calculations*** option

To perform *Petrological Calculations*, press the [***F7***] key from the Main Menu and a submenu will appear on the screen:

```
Mineral-Melt Geothermometers
     Fe3+/Fe2+ Ratios
     Water Solubility
      Special Tools
     Ternary Diagrams
```

Select one of the items using [↑] and [↓] keys and press [**Enter**].

*4.7.1. Mineral-Melt Geothermometers*

The INFOREX database has been primarily designed to provide access to published mineral-melt compositional information with the goal of developing empirical geothermometers, which in turn can be applied to the modeling of natural igneous systems (*Ariskin et al., 1987-1997*). To facilitate this function, the "*Mineral-Melt Geothermometers* " (*MMG*) option was incorporated into INFOREX which makes it possible to create a system of equations describing low pressure mineral-melt equilibria for rock-forming minerals such as olivine, plagioclase, high-Ca (augites from diopside to sub-calcium species) and low-Ca (pigeonite and orthopyroxene) pyroxenes as well as spinels (*Ariskin and Nikolaev, 1996*).

Following the extraction of a set of experimental data using INFOREX, including tables of coexisting mineral and glass compositions (e.g., see Fig. 13), the calibration of the equations is accomplished by multiple regression in the form of a modified Arrhenius relation:

$$\ln K_i = A / T + B \lg f_{O2} + C \ln R_{L1} + D \ln R_{L2} + E \ln R_{L3} + F, \qquad (1)$$

where $K_i$ is an equilibrium constant of a formation reaction, distribution coefficient or exchange constant for component-*i*, $T$ is the absolute temperature, $f_{O2}$ is oxygen fugacity, $R_{L1}$, $R_{L2}$, and $R_{L3}$ are the melt structure-chemical parameters, such as Si/O, NBO/T, Al/Si, (Na+K)/Al, $Fe^{3+}/Fe^{2+}$, etc., whereas the parameters *A, B, C, D, E,* and *F* are the regression constants.

To specify an equilibrium constant for the formation reaction (crystallization) of an end-member component, the degree to which $K_i$ is compositionally dependent could be determined as a function of the melt component activities. The INFOREX *MMG*-function enables the user to apply single oxide, two-lattice (*Nielsen and Dungan, 1983*) or a modified two-lattice model (*Ariskin and Barmina, 1990*) for the melt component activities calculations.

The use of melt structure chemical parameters as independent variables in the Equations (1) is a means to fine-tune the model. *This approach assumes that the effects of nonideality on mineral-melt equilibria can be attributed primarily to the liquid phase*.

The multiple linear regression calculations are build into the *MMG*-function, allowing the user to numerically study different combinations of equilibrium constants

versus reciprocal temperature, oxygen fugacity or melt structure-chemical parameters. After the regression parameters are calculated, the *MMG*-function calculates the statistics on goodness of fit by comparing the calculated and experimental values. This permits the user to independently estimate the accuracy of the geothermometers. If they do not satisfy the requirements for modeling, the calculations may be repeated for another combination of variables, until a good fit with the experimental data is obtained.

Working with the *MMG*-function

The *MMG* window includes 7 countered boxes with function keys abbreviations given at the bottom (Fig. 20). These boxes can be switched by the [***F3***] (***Next_Box***) key, with the exception of the 5th box when you are working with the *LIQUID PARAMETERS* mode (in such a case one should use the [***F5***] key to go to the following *REJECTING*-mode). In other cases the [***F5***] (***Browse***) key serves to view or print out initial datafiles and output files including the calculated parameters of mineral-melt geothermometers.

The [***F4***] (***Geotherm***) key is not active at the initial stage of working with *MMG*-function: it can be used to browse the **GEOTHERM.DAT** file (see below) only after completing the whole cycle of operations including specification of output files.

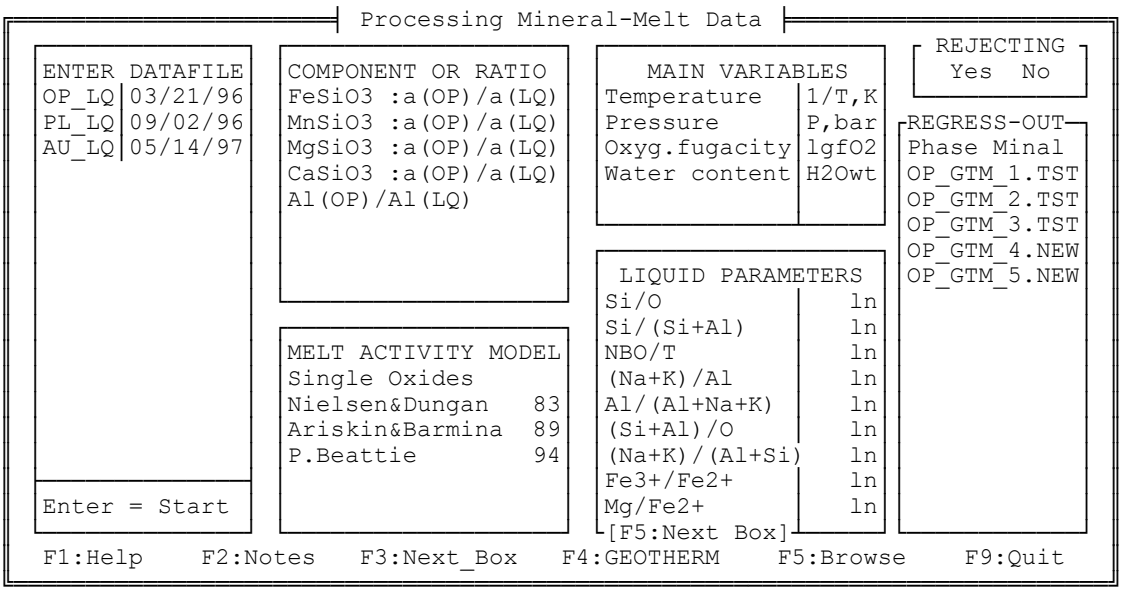



**Figure 20.** Screen image of the **Mineral-Melt Geothermometers** function
After completing operations for all 5 orthopyroxene end-members

**Note: After completing respective calculations (i.e., the creation of an output file) the [*F3*] (*Next_Box*) key is transformed to the [*F3*] (*New Calc.*) key which serves to come back to the first box in order to start calculations for another mineral-melt pair (if**

**desired). If you are going to continue work with same mineral, press the [*Shift+F3*] combination to come back to the *COMPONENT OR RATIO* box!**

```
OL 4
FeSi½O2:a(OL)/a(LQ)
MnSi½O2:a(OL)/a(LQ)
MgSi½O2:a(OL)/a(LQ)
CaSi½O2:a(OL)/a(LQ)
PL 4
FeAl2Si2O8:aPL/aLQ
CaAl2Si2O8:aPL/aLQ
NaAlSi3O8 :aPL/aLQ
KAlSi3O8  :aPL/aLQ
AU 5
FeSiO3 :a(AU)/a(LQ)
MnSiO3 :a(AU)/a(LQ)
MgSiO3 :a(AU)/a(LQ)
CaSiO3 :a(AU)/a(LQ)
Al(AU)/Al(LQ)
PG 5
FeSiO3 :a(PG)/a(LQ)
MnSiO3 :a(PG)/a(LQ)
MgSiO3 :a(PG)/a(LQ)
CaSiO3 :a(PG)/a(LQ)
Al(PG)/Al(LQ)
OP 5
FeSiO3 :a(OP)/a(LQ)
MnSiO3 :a(OP)/a(LQ)
MgSiO3 :a(OP)/a(LQ)
CaSiO3 :a(OP)/a(LQ)
Al(OP)/Al(LQ)
SP 5
FeCr2O4:a(SP)/a(LQ)
Cr/Al  :r(SP)/r(LQ)
Mg/Fe2+:r(SP)/r(LQ)
Fe3+/Fe2+(SP)
Ti(SP)/Ti(LQ)
MT 5
FeFe2O4:a(MT)/a(LQ)
Fe3/Ti :r(MT)/r(LQ)
Fe2TiO4:a(MT)/a(LQ)
Fe3+/Fe2+(MT)
Ti(MT)/Ti(LQ)
```

The left box in the *MMG* window always contains names and dates for files written in the “mineral-melt” format using the *SPA*-option (OP_LQ.DAT, PL_LQ.DAT, etc). One can select any file of interest by moving a highlighted field to the name desired using the arrow keys and pressing “Enter”. In response to this action a FORTRAN program will create an auxiliary file called COEXIST.DAT (Table 1) which will be used in further thermodynamic processing.

A list of end-member components for the designated mineral will appear in the second *COMPONENT OR RATIO* box (see the complete list to left). After selecting an end-member component, Al distribution coefficient, or a partition corfficient ratio one should specify *MELT ACTIVITY MODEL*: at this stage of the work with INFOREX we prefer to use the two-lattice model (*Nielsen and Dungan, 1983*) which was successfully used in the development of COMAGMAT (*Ariskin et al., 1993*) and METEOMOD (*Ariskin et al., 1997b*) phase equilibria models.

The third and fourth boxes serve to specify a set of parameters which can be used as independent variables in the least square fitting (see Eq. 1). The *MAIN VARIABLES* box allows one to include log$f_{O2}$ and total pressure (in bars) in the expressions being calibrated (reciprocal temperature *1/T,K* is always present), whereas the *LIQUID PARAMETERS* box includes logarithms of 9 melt structure-chemical ratios (*note, that one can add to the fitting simultaneously no more than 3 liquid parameters*).

After specification of the independent variables, press the [***F5***] key and indicate if you wish to activate a special *REJECTING* procedure (YES/NO). If YES, a message will appear on the screen asking for the maximum temperature deviation (precision of

calculations, $T_{exp}$-$T_{cal}$) if one is to use the calculated mineral-melt equilibria expressions as geothermometers:

```
Max.Temp. Deviation: ±2.00 σ
```

For example, typing 2.0 means that all experimental points for which calculated temperatures more than 2 times exceed in absolute value an average temperature deviations $T_{exp}$-$T_{cal}$ will be excluded from consideration at the next stage of thermodynamic processing.

*Structure of output files*

After calling for the REJECTING-procedure wait for a few seconds and results of the least square fitting will be displayed on the screen. Simultaneously an auxiliary file called REGRESS.OUT (Table 1) containing all of the independent variables will be created in the D:\INFOREX\SAVE directory:

| Numb | K3.dat | 1/Temp,K | Si/O | P(bar)/T,K | lg fO2 |
|---|---|---|---|---|---|
| 1 | .2465E+01 | .6481E-03 | .3172E+00 | .6481E-03 | -.7700E+01 |
| 2 | .1906E+01 | .6161E-03 | .3219E+00 | .6161E-03 | -.1120E+02 |
| 3 | .2035E+01 | .6246E-03 | .3200E+00 | .6246E-03 | -.1143E+02 |
| 4 | .2195E+01 | .6357E-03 | .3161E+00 | .6357E-03 | -.1173E+02 |
| 5 | .2197E+01 | .6357E-03 | .3183E+00 | .6357E-03 | -.1173E+02 |
| 6 | .2479E+01 | .6460E-03 | .3151E+00 | .6460E-03 | -.1201E+02 |
| 7 | .2945E+01 | .6698E-03 | .3040E+00 | .6698E-03 | -.1266E+02 |
| 8 | .3245E+01 | .6789E-03 | .3123E+00 | .6789E-03 | -.1290E+02 |
| 9 | .3480E+01 | .6882E-03 | .3250E+00 | .6882E-03 | -.1316E+02 |
| 10 | .3494E+01 | .6930E-03 | .3062E+00 | .6930E-03 | -.1332E+02 |
| 11 | .3729E+01 | .6930E-03 | .3258E+00 | .6930E-03 | -.1332E+02 |
| 12 | .2904E+01 | .6698E-03 | .3116E+00 | .6698E-03 | -.1266E+02 |
| 13 | .3137E+01 | .6789E-03 | .3165E+00 | .6789E-03 | -.1290E+02 |
| 14 | .3403E+01 | .6930E-03 | .3242E+00 | .6930E-03 | -.1332E+02 |

**Figure 21**. An example of REGRESS.OUT file used to develop *Opx*-melt expressions created from OP_LQ.DAT shown in Fig. 13

At this point, the program will ask if you wish to save the calculated parameters to GEOTHERM.DAT file (YES to save/"Enter" to skip) followed by a message asking to indicate the extension of output file to be created:

```
Enter file extension: TST
```

Examples of combined names of basic output files addressed to *Opx*-melt equilibrium are shown in Fig. 20 (note that digits "1","2",..."5" correspond to the number of an end-member component) .

```
2. Two Lattice Model by Nielsen,Dungan (1983)

Model fitting results for: MgSiO3
=========================================================
  Independent variables     Coefficient    Stand. error
=========================================================
      Constant                -4.18669          .38848
```

```
      1/Temp,K              8211.36300      245.97290
      ln Si/O                   .20300         .31863
=========================================================
  14 observations fitted

Numb lnK-Comp  10**4/T lnK(exp) lnK(cal)   D(lnK) T,C(exp) T,C(cal)   D(T,C)
   1   1.1353   6.4810    .9022    .9020    .0002   1270.0   1269.9       .1
   2    .8751   6.1610    .6450    .6422    .0028   1350.1   1349.2       .9
   3    .9418   6.2460    .7105    .7108   -.0003   1328.0   1328.1      -.1
   4   1.0200   6.3570    .7862    .7995   -.0133   1300.1   1304.1     -4.0
   5   1.0195   6.3570    .7871    .8009   -.0138   1300.1   1304.2     -4.2
   6   1.1423   6.4600    .9079    .8834    .0244   1275.0   1267.9      7.1
   7   1.3218   6.6980   1.0801   1.0716    .0085   1220.0   1217.7      2.3
   8   1.4134   6.7890   1.1771   1.1518    .0254   1200.0   1193.3      6.7
   9   1.4752   6.8820   1.2470   1.2362    .0108   1180.1   1177.3      2.8
  10   1.4913   6.9300   1.2510   1.2635   -.0125   1170.0   1173.2     -3.2
  11   1.5438   6.9300   1.3161   1.2761    .0400   1170.0   1159.9     10.1
  12   1.3028   6.6980   1.0661   1.0766   -.0105   1220.0   1222.8     -2.9
  13   1.3768   6.7890   1.1433   1.1545   -.0112   1200.0   1202.9     -3.0
  14   1.4533   6.9300   1.2247   1.2751   -.0505   1170.0   1182.9    -12.9
                     Average Deviations:    .0160                      4.3

ABS[lnK(exp)-lnK(cal)] <  STATISTICS > ABS[T(exp)-T(cal)]
     ± .05 - 92.9%                        ± 5.0° - 71.4%
     ± .10 -100.0%                        ±10.0° - 85.7%
     ± .15 -100.0%                        ±15.0° -100.0%
     ± .20 -100.0%                        ±20.0° -100.0%
     ± .25 -100.0%                        ±25.0° -100.0%
     ± .30 -100.0%                        ±30.0° -100.0%

Rejected:  11 D(Temp)=   10.1
Rejected:  14 D(Temp)=   12.9

Model fitting results for: MgSiO3
=========================================================
  Independent variables    Coefficient   Stand. error
=========================================================
      Constant               -4.15677         .27784
      1/Temp,K             8284.78900      201.46160
      ln Si/O                  .26996         .26930
=========================================================
  12 observations fitted

Numb lnK-Comp  10**4/T lnK(exp) lnK(cal)   D(lnK) T,C(exp) T,C(cal)   D(T,C)
   1   1.2122   6.4810    .9022    .9026   -.0004   1270.0   1270.1      -.1
   2    .9510   6.1610    .6450    .6415    .0035   1350.1   1349.0      1.1
   3   1.0181   6.2460    .7105    .7103    .0002   1328.0   1328.0       .1
   4   1.0971   6.3570    .7862    .7990   -.0128   1300.1   1303.9     -3.8
   5   1.0961   6.3570    .7871    .8008   -.0137   1300.1   1304.2     -4.1
   6   1.2196   6.4600    .9079    .8834    .0244   1275.0   1268.0      7.0
   7   1.4016   6.6980   1.0801   1.0709    .0092   1220.0   1217.5      2.5
   8   1.4913   6.7890   1.1771   1.1536    .0235   1200.0   1193.8      6.1
   9   1.5504   6.8820   1.2470   1.2414    .0056   1180.1   1178.6      1.4
  10   1.5705   6.9300   1.2510   1.2651   -.0140   1170.0   1173.5     -3.5
  12   1.3809   6.6980   1.0661   1.0776   -.0115   1220.0   1223.1     -3.1
  13   1.4538   6.7890   1.1433   1.1572   -.0139   1200.0   1203.6     -3.7
                     Average Deviations:    .0111                      3.1

ABS[lnK(exp)-lnK(cal)] <  STATISTICS > ABS[T(exp)-T(cal)]
     ± .05 -100.0%                        ± 5.0° - 83.3%
     ± .10 -100.0%                        ±10.0° -100.0%
     ± .15 -100.0%                        ±15.0° -100.0%
     ± .20 -100.0%                        ±20.0° -100.0%
     ± .25 -100.0%                        ±25.0° -100.0%
     ± .30 -100.0%                        ±30.0° -100.0%
```

**Figure 22**. An example of **OP_GTM_3.***** file developed with *MMG*-option two points were rejected after 1st stage of the thermodynamic processing

After completing the main *MMG* operations one can browse or print out the output files using the [***F5***] (***Browse***) key. The [***F4***] (***Geotherm***) key is now active allowing the user also to look at the GEOTHERM.DAT file which was changed if the

calculated regression parameters for a specified end-member component were written to the file (Fig. 23).

```
 LAM=2 Regr B     A/T,K lg(fO2) DV(bar) DV(H2O)  ln(LCP1)  ln(LCP2)  ln(LCP3)
PLAG: Kor=0.814 ============================================================
Fe   -10.235 14202.680    .000    .000    .000 -1.041(1)   .000(6)   .000(8)
An    -5.515 10121.080    .000    .000    .000   .000(1) -2.696(6)   .000(8)
Ab   -10.684 17056.690    .000    .000    .000   .000(1)   .000(6)   .000(8)
Or    -7.906 10561.180    .000    .000    .000   .000(1)   .000(6)   .000(8)
OLIV: Kca=0.033 ------------------------------------------------------------
Fa    -4.343  5951.826    .000    .000    .000  -.206(1)  -.559(2)   .000(8)
Mn    -6.161  6592.316    .000    .000    .000 -1.265(1)   .000(2)   .000(8)
Fo    -3.992  5623.459    .000    .000    .000  -.946(1)  -.798(2)   .000(8)
Ca    -6.931  5047.081    .000    .000    .000   .000(1)   .000(2)   .000(8)
AUG : Kal=0.240 ------------------------------------------------------------
Fs    -2.654  8638.068    .000    .000    .000  3.464(1)  -.832(2)   .000(1)
Mn    -5.367 11083.250    .000    .000    .000  2.528(1) -2.279(2)   .000(1)
En    -6.601 10247.640    .000    .000    .000  -.386(1)   .551(2)   .000(1)
Wo      .054   589.070    .000    .000    .000   .000(1)   .572(2)   .000(1)
PIG : Kal=0.115 ------------------------------------------------------------
Fs    -2.011  4628.454    .000    .000    .000  1.313(1) -1.219(2)   .000(1)
Mn     -.584  5009.566    .000    .000    .000  2.301(1)   .000(2)   .000(1)
En    -4.378  7820.873    .000    .000    .000  -.164(1)   .236(2)   .000(1)
Wo   -15.910 15087.660    .000    .000    .000 -4.165(1)  2.674(2)   .000(1)
OPX:  Kal=0.057 ------------------------------------------------------------
Fs    -3.296  4978.494    .000    .000    .000   .371(1) -1.014(2)   .000(8)
Mn      .202  2182.190    .000    .000    .000  2.153(1) -3.442(2)   .000(8)
En    -2.481  6256.046    .000    .000    .000   .743(1) -1.002(2)   .000(8)
Wo   -11.478 13457.620    .000    .000    .000  -.587(1)   .000(2)   .000(8)
SPIN: ???=0.000 ------------------------------------------------------------
FeCr2-14.598 43656.360   0.457    .000    .000 -6.514(2)   .000(1)  0.000(5)
Cr/Al -7.478 22277.570   0.267    .000    .000 -1.115(3)   .000(1)  0.000(5)
Mg/Fe-10.832 17996.040   0.581    .000      00 -3.203(2) -1.192(8)  0.000(5)
FE3/2-30.623 58107.130   2.007    .000    .000 -3.648(5) -3.026(8)  0.000(5)
K(Ti)-16.919 29209.050   0.840    .000    .000 -2.442(5) -1.731(8)  0.000(5)
============================================================================
```

**Figure 23**. An example of **GEOTHERM.DAT** file developed using the *MMG*-option for calibration of a numeric model describing phase equilibria in meteoritic igneous systems (*Ariskin et al., 1997b*)

The GEOTHERM.DAT file is a basic datafile used to calculate phase equilibria in mafic igneous systems by means of programs addressed to the COMAGMAT series (*Ariskin et al., 1993*). This ability to calculate mineral-melt geothermometers for a given range of conditions or compositions is one of the main advantages of the INFOREX database, in that the user can independently calibrate phase equilibria equations, test them and use in calculations of melting-crystallization relationships in the systems of interest .

*4.7.2. $Fe^{3+}/Fe^{2+}$ ratios*

An important parameter for magma differentiation models is the $Fe^{3+}/Fe^{2+}$ ratio in the magma. Several equations for these calculations have been proposed, with the dependence of Sack et al. (1980) being one of the most popular among igneous petrologists for the last 15 years . We have collected the initial experimental information on the $Fe^{3+}$-$Fe^{2+}$ redox equilibrium which is available in INFOREX including over 440 experiments. This makes it possible to test the proposed equations for a given range of oxygen fugacities or melt compositions, or even to independently develop numerical constraints on the empirical dependencies *(Nikolaev et al., 1996*).

The *Fe3+/Fe2+ ratios* function has been designed to calculate $Fe^{3+}/Fe^{2+}$ ratios in experimental glasses at a given temperature, oxygen fugacity ($lgf_{O2}$), and melt composition. Calculations can be conducted using one of nine empirical equations given below. Also, this function allows one to test the precision of these equations using data on direct $Fe^{3+}/Fe^{2+}$ ratio determinations in the melts (see example of RE_LQ.DAT file in Fig. 17).

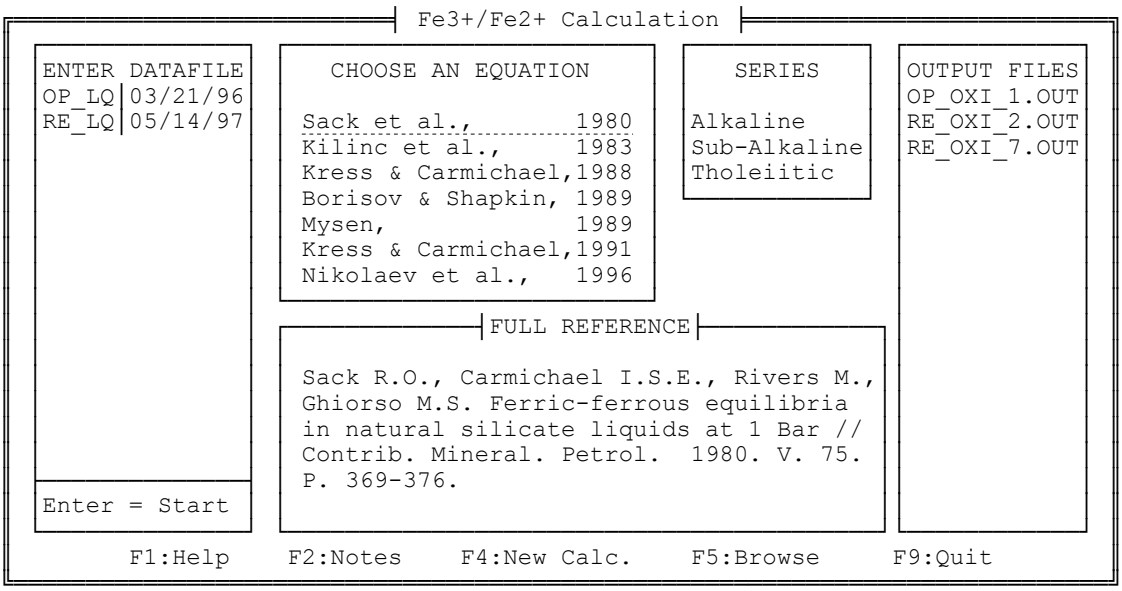



**Figure 24.** Screen image of the **Fe3+/Fe2+ RATIOS** calculation function
After work with OP_LQ.DAT and RE_LQ.DAT files

Working with the *Fe3+/Fe2+ ratios* function

The main *Fe3+/Fe2+ ratios* function window is configured in a way similar to *the Mineral-Melt Geothermometers* window and includes 5 boxes with the names of data files at the left side, and the names of output files at the right side (Fig. 24). Input files for the calculations are ****_LQ.DAT**, where double asterisk denotes RE, OP, LQ, OL, etc. Output files receive names such as ****_OXI_*.OUT**, where double asterisk denotes the same abbreviation as in the data file, whereas the character replacing single asterisk ranges from 1 to 9 depending on the calculation model selected.

There is no switching between the countered boxes: going from one box to another is done automatically after selection of a datafile or choice of an equation for the $Fe^{3+}/Fe^{2+}$ calculations. The [***F5***] (***Browse***) key serves to view or print out initial datafiles or output files including results of the calculations. The [***F4***] (***New Calc.***) key is not active at initial stage of working with the function. It can be used for repeating or conducting another set of calculations after specification of names of output files.

Basic Equation: Sack et al., 1980

| Numb | INFOREX Work | Run | P,kb EXP | Temp,C EXP | Temp,C CAL | lgfO2 EXP | lgfO2 CAL | lgfO2 δ(i) | Fe3+/Fe2+ EXP | Fe3+/Fe2+ CAL | Fe3+/Fe2+ δ(i) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 77 | 2 | .0 | 1270 | ND | -7.70 | ND | ND | ND | .109 | ND |
| 2 | 166 | 1 | .0 | 1350 | ND | -11.20 | ND | ND | ND | .009 | ND |
| 3 | 166 | 2 | .0 | 1328 | ND | -11.43 | ND | ND | ND | .009 | ND |
| 4 | 166 | 5 | .0 | 1300 | ND | -11.73 | ND | ND | ND | .009 | ND |
| 5 | 166 | 6 | .0 | 1300 | ND | -11.73 | ND | ND | ND | .009 | ND |
| 6 | 166 | 7 | .0 | 1275 | ND | -12.01 | ND | ND | ND | .010 | ND |
| 7 | 166 | 8 | .0 | 1220 | ND | -12.66 | ND | ND | ND | .010 | ND |
| 8 | 166 | 9 | .0 | 1200 | ND | -12.90 | ND | ND | ND | .011 | ND |
| 9 | 166 | 10 | .0 | 1180 | ND | -13.16 | ND | ND | ND | .012 | ND |
| 10 | 166 | 11 | .0 | 1170 | ND | -13.32 | ND | ND | ND | .011 | ND |
| 11 | 166 | 12 | .0 | 1170 | ND | -13.32 | ND | ND | ND | .013 | ND |
| 12 | 166 | 17 | .0 | 1220 | ND | -12.66 | ND | ND | ND | .010 | ND |
| 13 | 166 | 18 | .0 | 1200 | ND | -12.90 | ND | ND | ND | .011 | ND |
| 14 | 166 | 20 | .0 | 1170 | ND | -13.32 | ND | ND | ND | .012 | ND |

**Figure 25**. An example of **OP_OXI_1.OUT** file

The *Fe3+/Fe2+ ratios* function provides an access to nine basic equations proposed since 1980 (*note, that Nikolaev et al. proposed 3 different equations for the melts/magmas which could be addressed to tholeiitic, subalkaline, and alkaline series*):

*Structure of output files*

1. **Sack et al., 1980.**
2. **Kilinc et al., 1983.**
3. **Kress & Carmichael, 1988.**
4. **Borisov & Shapkin, 1989.**
5. **Mysen, 1989.**
6. **Kress & Carmichael, 1991.**
7. **Nikolaev et al., 1996 (for tholeiitic series).**
8. **Nikolaev et al., 1996 (for subalkaline series).**
9. **Nikolaev et al., 1996 (for alkaline series).**

Examples of output files which are created in the D:\INFOREX\SAVE directory are given in Figs 25-27: the column **Numb** includes successive numbers of the calculations; two columns addressed to the **INFOREX** section contain reference numbers (**Work**) and corresponding run numbers (**Run**); run pressure is given in the column **P,kb**, whereas experimental and calculated temperatures are in **EXP** and **CAL** columns of the **Temp,C** section.

Basic Equation: Kilinc et al., 1983

| Numb | INFOREX | | P,kb | Temp,C | | lgfO2 | | | Fe3+/Fe2+ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | Work | Run | | EXP | CAL | EXP | CAL | δ(i) | EXP | CAL | δ(i) |
| 1 | 152 | 1 | .0 | 1461 | 1405.7 | -7.17 | -6.69 | -.48 | .095 | .075 | .020 |
| 2 | 152 | 3 | .0 | 1459 | 1337.6 | -8.21 | -7.11 | -1.10 | .078 | .045 | .033 |
| 3 | 152 | 4 | .0 | 1459 | 1357.4 | -8.21 | -7.30 | -.91 | .070 | .044 | .026 |
| 4 | 152 | 6 | .0 | 1459 | 1295.3 | -9.21 | -7.69 | -1.52 | .059 | .027 | .032 |
| 5 | 152 | 11 | .0 | 1459 | 1368.9 | -6.15 | -5.35 | -.80 | .194 | .130 | .064 |
| 6 | 152 | 12 | .0 | 1459 | 1425.4 | -6.15 | -5.86 | -.29 | .156 | .135 | .021 |
| 7 | 152 | 20 | .0 | 1362 | 1325.4 | -7.93 | -7.58 | -.35 | .102 | .085 | .017 |
| 8 | 152 | 35 | .0 | 1366 | 1301.0 | -8.91 | -8.28 | -.63 | .062 | .045 | .017 |
| 9 | 152 | 38 | .0 | 1366 | 1354.2 | -8.91 | -8.80 | -.11 | .049 | .046 | .003 |
| 10 | 152 | 50 | .0 | 1363 | 1298.4 | -6.81 | -6.18 | -.63 | .189 | .137 | .052 |
| 11 | 152 | 51 | .0 | 1363 | 1300.5 | -6.81 | -6.20 | -.61 | .185 | .136 | .049 |
| σ=√(Σ(δ(i))²/n) | | | | | 84.2 | | | .77 | | | .035 |
| δ(av)=Σ\|δ(i)\|/n | | | | | 73.3 | | | .68 | | | .030 |

**Figure 26**. An example of **RE_OXI_1.OUT** file created from RE_LQ.DAT file given in Fig. 17

One can find experimental and calculated oxygen fugacities in the columns **EXP** and **CAL** of the **lgfO2** section (if the user intends to use the equations as oxybarometers). Differences between experimental and calculated values are placed in the field **δ(i)**=EXP-CAL. Experimental and calculated $FeO_{1.5}/FeO$ ratios are given in the columns **EXP** and **CAL** followed by the **δ(i)** = EXP-CAL value. If a parameter is unknown (there were no data in the reference source) the ND (*No Data*) index will appear in the corresponding field.

General statistics on the comparisons between experimental and calculated values for temperature, oxygen fugacity, and $Fe^{3+}/Fe^{2+}$ ratio is always given in the two lower rows: **σ=(Σ(δ(i))2/n)1/2** and **δ(av)=Σ|δ(i)|/n** (**av** - average).

Basic Equation: Nikolaev et al., 1996 (Tholeiitic)

| Numb | INFOREX | | P,kb | Temp,C | | lgfO2 | | | Fe3+/Fe2+ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | Work | Run | | EXP | CAL | EXP | CAL | δ(i) | EXP | CAL | δ(i) |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 152 | 1 | .0 | 1461 | 1518.0 | -7.17 | -7.60 | .43 | .095 | .109 | -.014 |
| 2 | 152 | 3 | .0 | 1459 | 1461.6 | -8.21 | -8.23 | .02 | .078 | .079 | -.001 |
| 3 | 152 | 4 | .0 | 1459 | 1497.6 | -8.21 | -8.51 | .30 | .070 | .077 | -.007 |
| 4 | 152 | 6 | .0 | 1459 | 1451.5 | -9.21 | -9.15 | -.06 | .059 | .058 | .001 |
| 5 | 152 | 11 | .0 | 1459 | 1380.6 | -6.15 | -5.51 | -.64 | .194 | .158 | .036 |
| 6 | 152 | 12 | .0 | 1459 | 1461.9 | -6.15 | -6.17 | .02 | .156 | .157 | -.001 |
| 7 | 152 | 20 | .0 | 1362 | 1422.2 | -7.93 | -8.44 | .51 | .102 | .120 | -.018 |
| 8 | 152 | 35 | .0 | 1366 | 1427.5 | -8.91 | -9.43 | .52 | .062 | .073 | -.011 |
| 9 | 152 | 38 | .0 | 1366 | 1533.4 | -8.91 | -10.24 | 1.33 | .049 | .075 | -.026 |
| 10 | 152 | 50 | .0 | 1363 | 1309.4 | -6.81 | -6.32 | -.49 | .189 | .162 | .027 |
| 11 | 152 | 51 | .0 | 1363 | 1302.9 | -6.81 | -6.26 | -.55 | .185 | .155 | .030 |
| $\sigma=\sqrt{(\Sigma(\delta(i))^2/n)}$ | | | | | 69.3 | | | .57 | | | .020 |
| $\delta(av)=\Sigma\lvert\delta(i)\rvert/n$ | | | | | 53.6 | | | .44 | | | .016 |

**Figure 27**. An example of **RE_OXI_7.OUT** file
If we examine the data of Fig. 26, one can see that the model of Nikolaev et al. (1996) works better than that of Kilinc et al. (1983)

**Note:** **As follows from the Figs 26 and 27 the *Fe3+/Fe2+ ratios* function can not only be used to test existing models calculating $Fe^{3+}/Fe^{2+}$ ratios in the melt, but also to calculate $lgf_{O2}$ values for melts with known $Fe^{3+}/Fe^{2+}$ ratios. To perform this operation one should create first an ASCII file like RE_LQ.DAT (see *the chapter 4.5*).**

### 4.7.3. *Water Solubility*

Another useful application of the INFOREX system is its ability to calculate water solubility in magmas. In the last decade, many investigations have been undertaken to develop thermodynamic models of water solubility. Each, to different extents, do so by accounting for the changes in the partial molar volume of $H_2O$ and for the relations between $H_2O$ species in silicate melts, see the review by *Holloway and Blank (1994).* One problem that we encounter in applying this information to natural systems is the fact that little experimental data on water solubility exists for natural systems, particularly for basalts and andesites. Therefore, a classic thermodynamic approach based on the use of independent constraints, such as the effect of temperature on the partial molar volume of $H_2O$, may generate additional errors to calculations of water solubility. Towards the end of producing useful, if empirical constraints, we have extracted the water solubility experiments from the INFOREX database to develop a purely empirical equation which can be applied to a wide range of systems and conditions (Almeev and Ariskin, 1996).

Processing of the data was carried out by multiple linear regression calculations with the melt structure-chemical parameters used as independent variables. A set of

17 parameter combinations were investigated. The best internal precision was obtained using the expression:

$$\ln(C_{H2O})_L = [-14710.2 + 38438.3(Si/O)_L](1/T) + 0.5868 \ln P - 21.455(Si/O)_L + 3.894(Al/Si)_L + 4.393, \quad (2)$$

where $(C_{H2O})_L$ is water content in silicate liquid (wt.%), $P$ is total pressure (bars), and Si/O and Al/Si are atomic ratios in the melt. Comparison of the experimental values with those calculated using the Equation (2) indicates an average accuracy of 0.3 wt.% $H_2O$; solving the inverse problem for pressure (if water content in a saturated melt is given) also indicates an average accuracy of 250 bars (Almeev and Ariskin, 1996). This is consistent with our current understanding of the strong effect of pressure on water solubility.

Derivation of the equation for the calculation of water solubility in magmatic melts shows how the information in the INFOREX database can be developed further. As mentioned above, there is a large existing dataset of water saturated experiments, but direct analytical information on the water contents in the experimental glasses is absent for almost all of them. To accomplish the goal we have implemented the *Water Solubility* function providing an access to 3 basic equations proposed and improved since 1979, including the above mentioned model of Almeev and Ariskin (1996):

1. **Burnham's model (1979-1994)**
2. **Stolper's model (1982-1995)**
3. **Almeev & Ariskin model (1996)**

The first function is based on the most recent Burnham's model parameters (*Burnham, 1994*), whereas the second one uses parameters of water solubility equation given by *Dixon et al. (1995)* with an algorithm provided by *Holloway and Blank (1994).*

Working with the *Water Solubility* function

The *Water Solubility* function window includes 5 boxes (Fig. 28). In the *ENTER DATAFILE* box one should select an initial datafile, containing information on the experimental conditions as well as quenched glasses compositions. These files are

implied to have been created earlier using the *SRC*- and *SPA*-options: they have names like ****_LQ.DAT**, where double asterisk denotes LQ, HB, OL, etc. The *CHOOSE A MODEL* box includes an ability to select a *Water Solubility* model (note the pressure restrictions given below at the box bottom - see Fig. 28). References for each model appear automatically in the *FULL REFERENCE* box accompanied by some additional comments. There is no switching between the countered boxes: going from one box to another is done automatically after pressing “Enter” to select a datafile or choose an equation for the water solubility calculations.

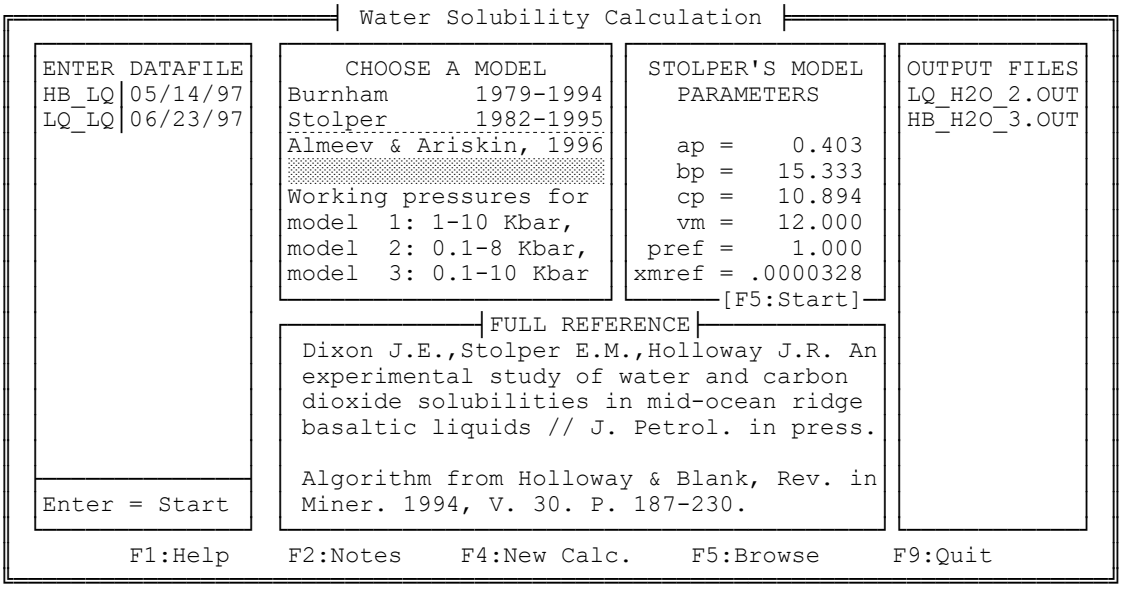



**Figure 28.** Screen image of the **Water Solubility** function
After work with LQ_LQ.DAT and HB_LQ.DAT files

The [***F5***] (***Browse***) key serves to display or print out initial datafiles or output files including results of the calculations. The [***F4***] (***New Calc.***) key is not active during the initial stage of working with the function: it can be used for repeating or conducting another set of calculations after specification of names of output files.

**Note: In contrast to other equations the Stolper's model requires few parameters you can change in the *STOLPER'S MODEL PARAMETERS* box - the default values for these parameters are taken from *Holloway and Blank (1994).***

*Structure of output files*

Output files receive names such as ****_H2O_*.OUT**, where double asterisk denotes the same abbreviation as in the data file, whereas the character replacing single asterisk ranges from 1 to 3 depending on the calculation model selected (Fig.

28). Examples of output files which are created in the D:\INFOREX\SAVE directory are given in Figs 29-30: the column **Numb** includes successive numbers of the calculations; two columns addressed to the **INFOREX** section contain reference numbers (**Work**) and corresponding run numbers (**Run**); **FLUID** column includes flags of the presence (*Yes*) or absence (*No*) of a vapor phase; run pressure and experimental temperature are given in the column **P,kb** and **Temp,C,** respectively. Experimental (if present) and calculated water contents are given the next 3 columns addressed to the **H2O solubility** title (Fig. 29).

Model for H2O solubility calculations: Almeev & Ariskin (1996)

| Numb | INFOREX | | FLUID | P,kb | Temp,C | H2O solubility | | |
|---|---|---|---|---|---|---|---|---|
| | Work | Run | | | | EXP | CAL | δ(i) |
| 1 | 111 | 36 | Yes | 2.0 | 800 | 5.95 | 6.05 | - |
| 2 | 111 | 66 | Yes | 2.0 | 1000 | 5.96 | 6.87 | - |
| 3 | 112 | 11 | Yes | 3.0 | 850 | ND | 7.98 | ND |
| 4 | 112 | 12 | Yes | 3.0 | 875 | ND | 7.61 | ND |
| 5 | 112 | 27 | Yes | 3.0 | 850 | ND | 8.16 | ND |
| 6 | 112 | 28 | Yes | 3.0 | 875 | ND | 7.91 | ND |
| 7 | 112 | 46 | Yes | 3.0 | 850 | ND | 7.92 | ND |
| 8 | 112 | 47 | Yes | 3.0 | 875 | ND | 7.64 | ND |
| 9 | 112 | 79 | Yes | 3.0 | 850 | ND | 7.95 | ND |
| 10 | 133 | 3 | Yes | 5.0 | 750 | ND | 11.59 | ND |
| 11 | 133 | 28 | Yes | 4.9 | 725 | ND | 12.29 | ND |
| 12 | 133 | 42 | Yes | 4.9 | 725 | ND | 12.18 | ND |
| 13 | 229 | 12 | Yes | 2.0 | 940 | ND | 6.35 | ND |

**Figure 29**. An example of **HB_H2O_2.OUT** file
Obtained from the HB_LQ.DAT file given in Fig. 16

In some cases water contents in experimental glasses were measured directly (in opposite to the water contents for the first two glasses of Work 111 which represent calculated values - Fig. 29). For such experiments, the *Water Solubility* function allows one to estimate the accuracy of the water contents calculations using 3 models considered above. To do this you should first choose the *H2O Content* - function of the *SRC*-option (see Fig. 11), followed by the *Only melt compositions + Melts Equilibrated with All Phases* functions of the *SPA*-option. These operations will result in the creation of a LQ_LQ.DAT file, including only glass compositions with measured $H_2O$ contents.

In such cases, the *Water Solubility* function calculates the difference between experimental and computed water contents placed in the field **δ(i)**. General statistics on the comparisons between experimental and calculated values is always present in the two lower rows: **σ=(Σ(δ(i))2/n)1/2** and **δ(av)=Σ|δ(i)|/n** (**av** - average) - see Fig. 30.

Model for H2O solubility calculations: Stolper (1982-1994)

| Numb | INFOREX Work | Run | FLUID | P,kb | Temp,C | H2O solubility EXP | CAL | δ(i) |
|---|---|---|---|---|---|---|---|---|
| 1 | 142 | 7 | Yes | 1.0 | 1100 | 4.49 | 3.36 | 1.13 |
| 2 | 142 | 8 | Yes | 2.0 | 1100 | 6.04 | 4.88 | 1.16 |
| 3 | 142 | 9 | Yes | 3.0 | 1100 | 7.40 | 6.15 | 1.25 |
| 4 | 142 | 10 | Yes | 4.0 | 1100 | 8.70 | 7.33 | 1.37 |
| 5 | 142 | 11 | Yes | 5.3 | 1100 | 10.08 | 8.82 | 1.26 |
| 6 | 201 | 20 | Yes | 1.0 | 1170 | 4.40 | 3.43 | .97 |
| 7 | 201 | 22 | Yes | 1.0 | 1100 | 4.50 | 3.38 | 1.12 |
| 8 | 201 | 24 | Yes | 1.0 | 1050 | 2.20 | 3.38 | -1.18 |
| 9 | 201 | 40 | Yes | 3.0 | 1030 | 6.50 | 5.93 | .57 |
| 10 | 201 | 45 | Yes | 3.0 | 1000 | 6.80 | 5.81 | .99 |
| 11 | 201 | 72 | Yes | 5.0 | 1100 | 8.80 | 8.52 | .28 |
| 12 | 201 | 79 | Yes | 5.0 | 1000 | 8.60 | 7.86 | .74 |
| 13 | 201 | 89 | Yes | 3.0 | 1200 | 5.65 | 6.48 | -.83 |
| 14 | 201 | 90 | Yes | 3.0 | 1200 | 5.62 | 6.48 | -.86 |
| 15 | 201 | 91 | Yes | 3.0 | 1100 | 6.53 | 6.18 | .35 |
| 16 | 201 | 92 | Yes | 3.0 | 1100 | 6.27 | 6.18 | .09 |

N of water saturated runs with directly determined H2O 16
σ=√(Σ(δ(i))²/N) .96
δ(av)=Σ|δ(i)|/N .89

**Figure 30**. An example of **LQ_H2O_2.OUT** file
Obtained from a LQ_LQ.DAT file including data on water solubility experiments in andesitic systems at 1 to 5 kbar pressures

### *4.7.4. Special Tools*

This is an additional option which permits one to perform some simple recalculations and formatting of the INFOREX data files created using the *SPA*-option. These 3 functions (Fig. 31) include:

1. Recast to 100% including $H_2O$ contents as follows:

   $\Sigma=SiO_2+TiO_2..+Cr_2O_3+H_2O$, $SiO_2'=100*(SiO_2/\Sigma)$, $TiO_2'=100*(TiO_2/\Sigma)$, etc.

   *Name of output file*: **RECAST_1.DAT** (Fig. 32)

2. Recast to 100% excluding $H_2O$ (dry residue) as follows:

   $\Sigma=SiO_2+TiO_2..+Cr_2O_3$, $SiO_2'=100*(SiO_2/\Sigma)$, $TiO_2'=100*(TiO_2/\Sigma)$, etc.

   *Name of output file*: **RECAST_2.DAT** (Fig. 33)

3. Creation of data files which permit the user to test mineral-melt geothermometers used to develop phase equilibria models, such as COMAGMAT (*Ariskin et al., 1993*) and METEOMOD (*Ariskin et al., 1997b*). This option replaces an INFOREX database number of an experiment in the melt composition row with the

value of experimental temperature. Such a file can be used without further reformatting in a special *Thermometry* mode of COMAGMAT and METEOMOD programs to compare calculated and experimental temperatures for each experimental point.

*Name of output file*: ****_THMEQ.DAT** (Fig. 34)

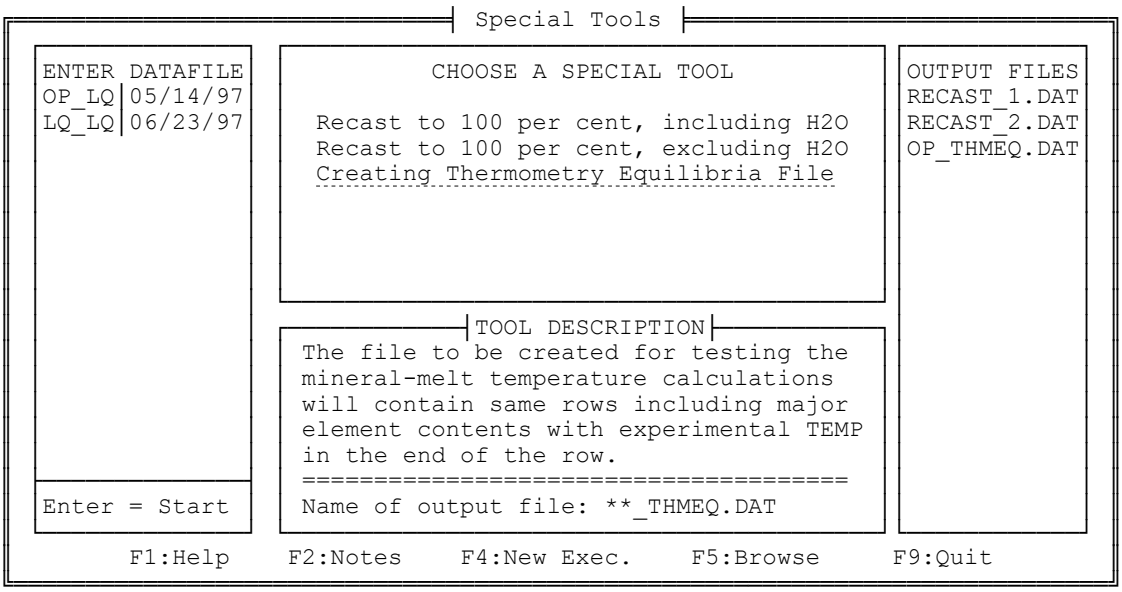



**Figure 31.** Screen image of the **Special Tools** function
After work with LQ_LQ.DAT and OP_LQ.DAT files

| SiO2 | TiO2 | Al2O3 | FeO | MnO | MgO | CaO | Na2O | K2O | P2O5 | Cr2O3 | H2O | N | n |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 56.04 | 1.10 | 17.51 | 6.05 | 0.10 | 3.25 | 6.43 | 4.17 | 0.79 | 0.25 | 0.00 | 4.31 | 142 | 7 |
| 55.22 | 1.09 | 17.25 | 5.97 | 0.09 | 3.20 | 6.33 | 4.11 | 0.78 | 0.25 | 0.00 | 5.71 | 142 | 8 |
| 54.52 | 1.07 | 17.03 | 5.89 | 0.09 | 3.16 | 6.25 | 4.06 | 0.77 | 0.24 | 0.00 | 6.91 | 142 | 9 |
| 53.86 | 1.06 | 16.83 | 5.82 | 0.09 | 3.13 | 6.18 | 4.01 | 0.76 | 0.24 | 0.00 | 8.02 | 142 | 10 |
| 53.19 | 1.05 | 16.62 | 5.75 | 0.09 | 3.09 | 6.10 | 3.96 | 0.75 | 0.24 | 0.00 | 9.18 | 142 | 11 |
| 56.80 | 0.49 | 18.58 | 4.34 | 0.08 | 2.48 | 7.31 | 3.96 | 1.53 | 0.17 | 0.00 | 4.25 | 201 | 20 |
| 56.75 | 0.49 | 18.56 | 4.34 | 0.08 | 2.48 | 7.30 | 3.96 | 1.53 | 0.17 | 0.00 | 4.35 | 201 | 22 |
| 60.56 | 0.53 | 18.10 | 3.49 | 0.11 | 2.77 | 6.86 | 3.65 | 1.66 | 0.00 | 0.02 | 2.25 | 201 | 24 |
| 55.67 | 0.48 | 18.21 | 4.25 | 0.08 | 2.43 | 7.16 | 3.88 | 1.50 | 0.17 | 0.00 | 6.16 | 201 | 40 |
| 55.52 | 0.48 | 18.16 | 4.24 | 0.08 | 2.43 | 7.14 | 3.87 | 1.49 | 0.17 | 0.00 | 6.42 | 201 | 45 |
| 54.49 | 0.47 | 17.82 | 4.16 | 0.07 | 2.38 | 7.01 | 3.80 | 1.46 | 0.17 | 0.00 | 8.16 | 201 | 72 |
| 54.59 | 0.47 | 17.85 | 4.17 | 0.07 | 2.39 | 7.02 | 3.81 | 1.47 | 0.17 | 0.00 | 7.99 | 201 | 79 |
| 56.13 | 0.49 | 18.36 | 4.29 | 0.08 | 2.45 | 7.22 | 3.92 | 1.51 | 0.17 | 0.00 | 5.40 | 201 | 89 |
| 56.14 | 0.49 | 18.36 | 4.29 | 0.08 | 2.46 | 7.22 | 3.92 | 1.51 | 0.17 | 0.00 | 5.37 | 201 | 90 |
| 55.66 | 0.48 | 18.20 | 4.25 | 0.08 | 2.43 | 7.16 | 3.88 | 1.50 | 0.17 | 0.00 | 6.18 | 201 | 91 |
| 55.80 | 0.48 | 18.25 | 4.26 | 0.08 | 2.44 | 7.18 | 3.89 | 1.50 | 0.17 | 0.00 | 5.95 | 201 | 92 |

**Figure 32**. An example of **RECAST_1.DAT** file
Obtained from the LQ_LQ.DAT used to demonstrate calculations in Figs 28 and 30

| SiO2 | TiO2 | Al2O3 | FeO | MnO | MgO | CaO | Na2O | K2O | P2O5 | Cr2O3 | H2O | N | n |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 58.56 | 1.15 | 18.30 | 6.33 | 0.10 | 3.40 | 6.72 | 4.36 | 0.82 | 0.26 | 0.00 | 0.00 | 142 | 7 |
| 58.56 | 1.15 | 18.30 | 6.33 | 0.10 | 3.40 | 6.72 | 4.36 | 0.82 | 0.26 | 0.00 | 0.00 | 142 | 8 |
| 58.56 | 1.15 | 18.30 | 6.33 | 0.10 | 3.40 | 6.72 | 4.36 | 0.82 | 0.26 | 0.00 | 0.00 | 142 | 9 |
| 58.56 | 1.15 | 18.30 | 6.33 | 0.10 | 3.40 | 6.72 | 4.36 | 0.82 | 0.26 | 0.00 | 0.00 | 142 | 10 |
| 58.56 | 1.15 | 18.30 | 6.33 | 0.10 | 3.40 | 6.72 | 4.36 | 0.82 | 0.26 | 0.00 | 0.00 | 142 | 11 |
| 59.33 | 0.51 | 19.40 | 4.53 | 0.08 | 2.59 | 7.63 | 4.14 | 1.59 | 0.18 | 0.00 | 0.00 | 201 | 20 |

```
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 22
61.95  0.54 18.52  3.57  0.11  2.83  7.02  3.74  1.70  0.00  0.02  0.00 201 24
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 40
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 45
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 72
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 79
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 89
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 90
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 91
59.33  0.51 19.40  4.53  0.08  2.59  7.63  4.14  1.59  0.18  0.00  0.00 201 92
```

**Figure 33**. An example of **RECAST_2.DAT** file
Obtained from the LQ_LQ.DAT used to demonstrate calculations in Figs. 28 and 30

Both RECAST_1.DAT and RECAST_2.DAT can be further used in graphics plotting programs, whereas contents of major elements in the **_THMEQ.DAT still needed to be recast to 100%.

| SiO2 | TiO2 | Al2O3 | FeO | MnO | MgO | CaO | Na2O | K2O | P2O5 | Cr2O3 | H2O | T obs°C |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 50.47 | 0.98 | 7.98 | 17.38 | 0.56 | 10.98 | 9.52 | 0.70 | 0.00 | 0.00 | 0.27 | 0.00 | 1270 |
| 52.10 | 0.23 | 5.64 | 23.30 | 0.44 | 14.60 | 4.52 | 0.01 | 0.00 | 0.00 | 0.74 | 0.00 | 1350 |
| 50.90 | 0.26 | 6.48 | 23.20 | 0.42 | 12.90 | 5.12 | 0.02 | 0.00 | 0.00 | 0.77 | 0.00 | 1328 |
| 50.60 | 0.29 | 7.21 | 24.30 | 0.40 | 12.10 | 5.69 | 0.01 | 0.00 | 0.00 | 0.77 | 0.00 | 1300 |
| 50.80 | 0.28 | 6.95 | 24.50 | 0.41 | 11.80 | 5.50 | 0.03 | 0.00 | 0.06 | 0.70 | 0.00 | 1300 |
| 50.60 | 0.38 | 8.50 | 23.40 | 0.41 | 10.40 | 6.85 | 0.03 | 0.00 | 0.07 | 0.72 | 0.00 | 1275 |
| 48.90 | 0.44 | 11.90 | 21.20 | 0.35 | 8.54 | 8.59 | 0.03 | 0.00 | 0.40 | 0.44 | 0.00 | 1220 |
| 50.70 | 0.47 | 13.00 | 17.80 | 0.32 | 7.31 | 8.39 | 0.69 | 0.00 | 0.52 | 0.38 | 0.00 | 1200 |
| 53.80 | 0.44 | 13.50 | 16.00 | 0.27 | 6.13 | 8.16 | 1.29 | 0.00 | 0.16 | 0.27 | 0.00 | 1180 |
| 49.60 | 0.50 | 14.80 | 16.80 | 0.30 | 6.70 | 10.10 | 0.12 | 0.00 | 0.14 | 0.29 | 0.00 | 1170 |
| 54.20 | 0.45 | 14.00 | 15.00 | 0.27 | 5.80 | 8.00 | 1.58 | 0.00 | 0.36 | 0.22 | 0.00 | 1170 |
| 49.10 | 0.35 | 9.47 | 24.60 | 0.30 | 7.97 | 7.84 | 0.05 | 0.00 | 0.20 | 0.43 | 0.00 | 1220 |
| 50.80 | 0.40 | 11.10 | 22.00 | 0.29 | 6.85 | 8.11 | 0.33 | 0.00 | 0.14 | 0.43 | 0.00 | 1200 |
| 52.90 | 0.42 | 12.10 | 18.60 | 0.24 | 5.79 | 8.64 | 1.01 | 0.00 | 0.19 | 0.27 | 0.00 | 1170 |

**Figure 34**. An example of **OP_THMEQ.DAT** file
Obtained from the OP_LQ.DAT shown in Fig. 13

**Note:** **In contrast to the *Fe3+/Fe2+ ratios* and *Water Solubility* functions, the [*F4*] key in the *Special Tools* function window is labeled as *New Exec:* in fact this is same as *New Calc.***

### *4.7.5. Ternary Diagrams*

One of traditional techniques of the use of melting-experiment information is to project experimental glass compositions onto ternary diagrams, such as *AFM* (alkalis-

FeO-MgO), *OLIV-CPX-QTZ*, or *AB-AN-QTZ*. Despite the fact that such a projection results in the lost of a part of potentially important chemical information, many scientists still use that approach for making comparisons of natural glasses (rocks, inclusions) compositions with those obtained in experiments. To make this work easier and faster we have developed the *Ternary Diagrams* function which allows one to calculate the projection parameters based on the techniques of Grove (*Tormey et al., 1987; Grove, 1993*) and *Walker et al. (1979)*.

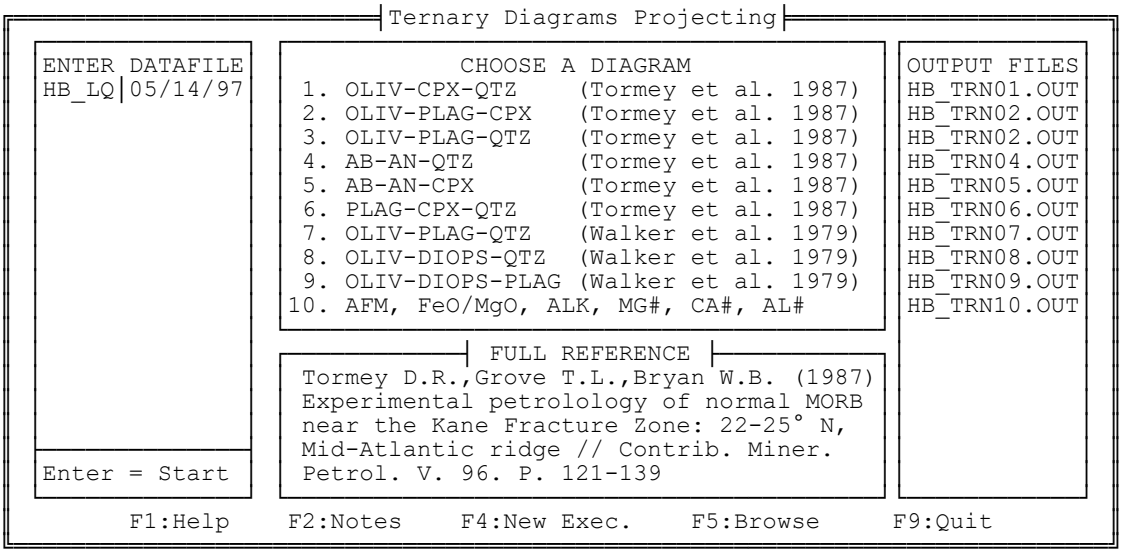



**Figure 35.** Screen image of the **Ternary Diagrams** function
After work with HB_LQ.DAT file

Working with the *Ternary Diagrams* function

The *Ternary Diagrams* function window includes 5 boxes (Fig. 35), similar to the *Special Tools* function window (Fig. 31). In the *ENTER DATAFILE* box one can select an initial datafile, whereas output files are displayed in the right *OUTPUT FILES* box. There is no switching between the countered boxes: going from one box to another is done automatically after pressing “Enter” to select a datafile or choose a type of ternary diagram for which the projection parameters will be calculated.

*Structure of output files*

Output files receive names such as ****_TRN**.OUT**, where the first double asterisk denotes the same abbreviation as in the data file, whereas the second ranges from 01 to 10 depending on the ternary diagram selected (Fig. 35). Examples of output files which are created in the D:\INFOREX\SAVE directory are given in Figs. 36-38.

For the files named ****_TRN01.OUT** to ****_TRN09.OUT** the column **Numb** includes successive numbers of the calculations, two columns addressed to the **INFOREX** section contain reference numbers (**Work**) and corresponding run numbers (**Run**), **Temp,C** column contains the value of experimental temperature; the next 3 columns include the calculated projection parameters followed with norms in oxygen units.

1 Ol#,CPx#,Qtz# - projection parameters for Ol-CPx-Qtz ternary

Oxygen units(%) from Tormey et al.,1987

| Numb | INFOREX Work | Run | TempC | Ol# | CPx# | Qtz# | QTZ | PLAG | OLIV | CPX | OXIDE | ORT | AP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 111 | 36 | 800 | .068 | -.011 | .944 | 25.4 | 54.0 | 1.8 | -.3 | .5 | 18.5 | .0 |
| 2 | 111 | 66 | 1000 | .088 | .083 | .828 | 14.8 | 72.9 | 1.6 | 1.5 | 3.1 | 6.1 | .0 |
| 3 | 112 | 11 | 850 | .074 | -.213 | 1.139 | 49.2 | 48.5 | 3.2 | -9.2 | 2.7 | 5.4 | .2 |
| 4 | 112 | 12 | 875 | .081 | -.196 | 1.115 | 43.5 | 52.8 | 3.1 | -7.6 | 3.0 | 4.8 | .3 |
| 5 | 112 | 27 | 850 | .108 | -.319 | 1.212 | 47.3 | 57.3 | 4.2 | -12.5 | 2.7 | .6 | .2 |
| 6 | 112 | 28 | 875 | .108 | -.312 | 1.204 | 36.1 | 66.3 | 3.2 | -9.3 | 2.8 | .5 | .4 |
| 7 | 112 | 46 | 850 | .082 | -.219 | 1.137 | 50.9 | 49.2 | 3.7 | -9.8 | 2.9 | 2.9 | .2 |
| 8 | 112 | 47 | 875 | .081 | -.203 | 1.122 | 42.3 | 56.7 | 3.1 | -7.7 | 2.9 | 2.3 | .4 |
| 9 | 112 | 79 | 850 | .080 | -.245 | 1.165 | 41.3 | 53.4 | 2.9 | -8.7 | 2.4 | 8.5 | .3 |
| 10 | 133 | 3 | 750 | .081 | -.164 | 1.083 | 42.0 | 51.0 | 3.1 | -6.4 | .4 | 9.9 | .0 |
| 11 | 133 | 28 | 725 | .087 | -.210 | 1.123 | 48.8 | 43.2 | 3.8 | -9.1 | .3 | 13.1 | .0 |
| 12 | 133 | 42 | 725 | .061 | -.163 | 1.102 | 47.8 | 42.5 | 2.6 | -7.1 | 1.1 | 13.0 | .0 |
| 13 | 229 | 12 | 940 | .042 | .188 | .771 | 9.9 | 73.2 | .5 | 2.4 | 2.4 | 11.6 | .0 |

**Figure 36**. An example of **HB_TRN01.OUT** file
Obtained from the HB_LQ.DAT shown in Fig. 16

2 Ol#,Pl#,Qtz# - projection parameters for Ol-Pl-Qtz ternary

Oxygen units(%) from Walker et al.,1979

| Numb | INFOREX Work | Run | TempC | Ol# | Pl# | Qtz# | QTZ | PLAG | OLIV | DIOPS |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 111 | 36 | 800 | .024 | .408 | .568 | 56.9 | 40.9 | 2.4 | -.2 |
| 2 | 111 | 66 | 1000 | .054 | .559 | .387 | 38.2 | 55.1 | 5.4 | 1.4 |
| 3 | 112 | 11 | 850 | .039 | .211 | .750 | 78.6 | 22.1 | 4.1 | -4.8 |
| 4 | 112 | 12 | 875 | .043 | .245 | .713 | 74.1 | 25.4 | 4.4 | -4.0 |
| 5 | 112 | 27 | 850 | .046 | .228 | .725 | 77.4 | 24.3 | 5.0 | -6.7 |
| 6 | 112 | 28 | 875 | .045 | .311 | .644 | 67.9 | 32.8 | 4.8 | -5.5 |
| 7 | 112 | 46 | 850 | .042 | .199 | .758 | 79.6 | 20.9 | 4.4 | -5.0 |
| 8 | 112 | 47 | 875 | .041 | .254 | .704 | 73.2 | 26.5 | 4.3 | -4.0 |
| 9 | 112 | 79 | 850 | .037 | .268 | .695 | 72.8 | 28.1 | 3.9 | -4.8 |
| 10 | 133 | 3 | 750 | .029 | .259 | .712 | 73.9 | 26.9 | 3.0 | -3.7 |
| 11 | 133 | 28 | 725 | .031 | .217 | .752 | 78.9 | 22.8 | 3.2 | -4.9 |
| 12 | 133 | 42 | 725 | .027 | .221 | .753 | 78.2 | 22.9 | 2.8 | -3.9 |
| 13 | 229 | 12 | 940 | .037 | .676 | .287 | 28.0 | 66.0 | 3.6 | 2.5 |

**Figure 37**. An example of **HB_TRN07.OUT** file
Obtained from the HB_LQ.DAT shown in Fig. 16

First 4 columns in the file ****_TRN10.OUT** are the same as in other output files, whereas next 9 columns contain 3 projection parameters for the *AFM* diagram followed by 6 additional routinely used petrochemical coefficients and ratios.

3 A#, F#, M# - projection parameters for AFM ternary diagram
ALK - Na2O+K2O; MG# - Mg/(Mg+Fe*); Ca# - Ca/(Ca+Al); AL# - (Na+K)/Al

| Numb | INFOREX Work | Run | TempC | A# | F# | M# | SiO2 wt% | FeO/MgO wt | ALK wt% | MG# mol | CA# mol | AL# mol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 111 | 36 | 800 | .825 | .132 | .042 | 67.04 | 3.14 | 8.23 | .362 | .079 | .819 |
| 2 | 111 | 66 | 1000 | .594 | .306 | .099 | 53.54 | 3.09 | 4.85 | .366 | .245 | .385 |
| 3 | 112 | 11 | 850 | .649 | .308 | .044 | 74.37 | 7.04 | 3.71 | .202 | .155 | .343 |
| 4 | 112 | 12 | 875 | .614 | .300 | .086 | 71.85 | 3.48 | 3.99 | .339 | .176 | .358 |
| 5 | 112 | 27 | 850 | .670 | .289 | .041 | 74.13 | 7.00 | 3.89 | .203 | .113 | .371 |
| 6 | 112 | 28 | 875 | .706 | .253 | .041 | 70.16 | 6.14 | 4.81 | .225 | .147 | .419 |
| 7 | 112 | 46 | 850 | .573 | .348 | .079 | 74.29 | 4.40 | 3.11 | .289 | .165 | .297 |
| 8 | 112 | 47 | 875 | .627 | .295 | .077 | 71.63 | 3.82 | 3.97 | .318 | .177 | .364 |
| 9 | 112 | 79 | 850 | .758 | .224 | .018 | 72.68 | 12.67 | 5.15 | .123 | .134 | .445 |
| 10 | 133 | 3 | 750 | .000 | .000 | .000 | 74.40 | .00 | 5.50 | .000 | .126 | .502 |
| 11 | 133 | 28 | 725 | .000 | .000 | .000 | 75.80 | .00 | 4.80 | .000 | .123 | .414 |
| 12 | 133 | 42 | 725 | .818 | .175 | .007 | 76.00 | 26.75 | 5.00 | .062 | .133 | .449 |
| 13 | 229 | 12 | 940 | .709 | .262 | .029 | 60.29 | 8.97 | 7.04 | .166 | .221 | .487 |

**Figure 38**. An example of **HB_TRN10.OUT** file
Obtained from the HB_LQ.DAT shown in Fig. 16

# Chapter 5. Troubleshooting

## *5.1. Memory problems*

The most common problem you can encounter working with the INFOREX database is memory problems. These problems look like INFOREX "does not want to work" with the *SCR-*, *SPA-,* or *Petrological Calculations* options. This is due to the fact that the INFOREX database needs at least 590K conventional memory (see *the chapter 1.2*). However, often the users have too many resident programs stored in the memory to run the system properly. To avoid this problem, we recommend that you make sure there is enough conventional memory on your computer before starting INFOREX.

To do this type in the DOS command line **mem /c /p** and a message on the screen will provide you a complete information on the distribution of conventional memory between resident programs and free memory available.

All is well if there is more than 590K free conventional memory. If not, one should make some arrangements in the computer configuration.

1. If you are working under **DOS 5.0** or higher, just use the **MEMMAKER.EXE** program in ..\DOS directory to improve your computer memory allocation (follow all of the instructions appeared on the screen). Use the command **mem /c /p** to make sure you have accomplished the goal.

If there is still not enough memory after the *memmaker.exe operations*, one should make changes in your **AUTOEXEC.BAT** file to free some additional memory.

Contact a technician to do that (in such a case it is convenient to have 2 copies of AUTOEXEC.BAT files with one of them addressed to the use of the INFOREX database).

2. If you are working with DOS emulated from **WINDOWS 95** or higher, it is also necessary to make changes in the **AUTOEXEC.BAT** and **CONFIG.SYS** files. A simple example of these files is given below (the main idea is to load as many programs into the upper memory as possible). If you use another programs you can load them like given in these examples.

**AUTOEXEC.BAT:**

```
@echo off
PATH=C:\WINDOWS;C:\WINDOWS\COMMAND
SET TMP=D:\TMP
mode con codepage prepare=((866) C:\WINDOWS\COMMAND\ega3.cpi)
mode con codepage select=866
```

**CONFIG.SYS:**

```
DEVICE=C:\WINDOWS\HIMEM.SYS
DEVICEHIGH=C:\WINDOWS\EMM386.EXE RAM
DEVICEHIGH=C:\WINDOWS\COMMAND\display.sys con=(ega,,1)
INSTALLHIGH=C:\WINDOWS\COMMAND\NLSFUNC.EXE C:\WINDOWS\COMMAND\COUNTRY.SYS
Country=007,866,C:\WINDOWS\COMMAND\country.sys
DOS=HIGH
DOS=UMB
BUFFERS=15,0
FILES=30
```

3. There are should not be any memory problems if you are working under **OS/2 Merlin**, in that it provides 610K free memory automatically without a special configuration.

### *5.2. Correction of mismatch problems*

In the case of mismatch problems encountered during *SPA* operations (working with the *Mineral-Melt Equilibria* or *Two mineral equilibria* functions), a message on the creation of a **BASE.ERR** file appears on the screen. This auxiliary file is located in the D:\INFOREX\SAVE\.. directory and includes a set of strings addressed to the INFOREX numbers of experiments where these errors were detected. These strings are formatted

in the CONDIT.EXP fashion (see Fig. 3) with the detected errors being usually caused by mismatches in the phase assemblages flags. For example, if index OL1 is given there while the olivine composition for same experiment is absent in the OLIV.EXP file.

To correct the problem the user must write the INFOREX database numbers of experiments where these errors were detected and run INFOREX again. Using the *Browse* function of the *GSI* option one should examine the mineral composition file which was involved in the *Mineral-Melt Equilibria* or *Two mineral equilibria* processing in detail.

After determining what compositions are absent, the user must return to the *Main Menu*, select the *V/E/I* option and using the [***F2***] (**Go to**) key to call for the study considered. Press the [***F4***] (***Edit***) function key to initialize the *Edit* function, and correct the corresponding strings of run conditions by deleting the mistaken symbols <1>. Press the [***F3***] (***Next***) key to call for a function to save the changes (see *the chapter 4.3.2*). After that, one should repeat the search process beginning from the *SRC*-option followed by SPA-functions of interest. These operations need to be done until the BASE.ERR file is empty.

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# Appendix 1

## *On-line help (HELP.TXT file)*

```
26 25
                    On-Line Help Facility                                  1

          INFOREX EXPERIMENTAL DATABASE (Ver. 4.0, 1997)
           Copyright (C) 1991-97. All rights reserved.
          A.A.Ariskin and S.S.Meshalkin (Moscow, Russia)

      INFOREX is a sophisticated manager for igneous petrologists and
   geochemists interested in the use of experimental information on
   phase equilibria in molten silicate systems. It is designed as an
   aid in searching the published experimental data, and extracting
   specific subsets of that data.

      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. In addition, the program allows one to derive numerical mineral-melt equilibria expressions (geothermometers) based on any data set.

INFOREX is hot-key driven, allowing users to easily and quickly sort through the data using any set of experimental conditions or rock type parameters. There are 7 main INFOREX options including:

Esc - exit PgDn

26 25

On-Line Help Facility 2

| | | |
|---|---|---|
| <F1> | System Configuration | [ SC ] |
| <F2> | General System Information | [ GSI ] |
| <F3> | View/Edit/Input data files | [ V/E/I ] |
| <F4> | Selecting Run Conditions | [ SRC ] |
| <F5> | Selecting Phase Assemblage | [ SPA ] |
| <F6> | Exchange INFOREX Data | [ EID ] |
| <F7> | Petrological Calculations | [ PC ] |
| <F9> | Quit | |

SC - includes an utility to change INFOREX settings, such as PATHS, PHASES, SYSTEMS, CONTAINERS, etc.

GSI - allows the user to receive General System Information on the current state of the INFOREX database as well as to browse basic data files on the screen.

V/E/I - provides operations for VIEWing, EDITing, and INPUT (updating) of the database files. It includes also an ability to write master records to a file or print them out.

SRC - permits one to Specify Run Conditions, such as rock types plus a range of pressures, temperatures, fO2, and melt compositions.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 3

SPA - allows the user to Select Phase Assemblages and to create phase equilibria compositional datafiles corresponding to the previously selected set of experiments (see the SRC-option). These files can be used in further thermodynamic processing.

EID - provides Export/Import operations including an ability to write results of new experimental studies directly to INFOREX database or save information under a given reference to a separate file.

PC - includes 5 kinds of Petrological Calculations, such as:

1. Creation of Mineral-Melt equilibria geothermometers;
2. Computation Fe3+/Fe2+ ratios for the experimental glasses;
3. Estimates of Water Solubility for the experimental glasses produced in water-saturated experiments;
4. Special Tools, including creation of files for testing of the COMAGMAT and METEOMOD phase equilibria models;
5. Computations of projection parameters for Ternary Diagrams routinely used in petrology.

QUIT - same as ESC, back 1 level.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 4

GENERAL SYSTEM INFORMATION

If you used the <F2> function key in the MAIN MENU you should wait for the program to read database information.

The available data base parameters will appear on the screen and further actions in GSI routine can be initiated using function keys keys or cursor:

Using the Function Keys in GSI-Routine

F1: Help - displays all specific options of the INFOREX system and always is the same as in MAIN MENU.

F2: Notes - involves 5 pages with tables deciphering indices, search words and flags used in the database.

F3: Save - saves a copy of the GSI screen in the 'general.inf' file on '\INFOREX\SAVE\' disk directory.

F4: Print  - prints the current text screen on the printer.
F5: Browse - permits browsing of any INFOREX database files.
F9: Quit   - same as ESC, quits the current operation.

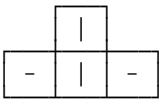
Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 5

To browse the INFOREX system database files press <F5> key and select "Phase compositions"/"Run conditions"/"References" highlighted field using the cursor and the "Enter" key.

If you selected the "Phase compositions" mode you must select a desired compositional file using the cursor keys located on the right-hand keypad.
Move the highlighted field to file name and and press "Enter".



VIEW/EDIT/INPUT DATA FILES

The V/E/I-routine screen is always divided on two windows with a reference in the upper part. One can scan the 'bibl.txt' reference file here using "PageDn" or "PageUp" keys.
If you need to quickly find a reference based on its number, use the <F2> function key. To change a mode of the routine, press <F3> or <F4> function keys.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 6

Using the Function Keys in VIEW/EDIT-modes

F1: Help   - displays all specific options of the INFOREX system and always is the same as in MAIN MENU.
F2: Goto   - allows you to leave or come back to a reference by means of scanning the reference list.
F3: Input  - calls INPUT mode.
F4: Edit   - calls EDIT mode.
F5: Write  - writes to a file on '\INFOREX\SAVE\' disk directory or prints on printer if type 'PRN' instead of a file name.
F9: Quit   - same as ESC, quits the current operation.

To browse or edit information concerning a given experimental study in V/E modes, press "Enter" and wait for a few seconds until 'condit__.exp' file data appear in the lower window. To scan this file use "PageDn" or "PageUp" keys (see next page). To make changes in the selected study information press <F4> and move a highlighted field to the field of interest with arrow keys. Make changes and press "Enter".

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 7

Note, that after pressing "Enter" at a selected reference the current meaning of the <F2> key will be transformed to "Notes" and the <F3> key will be transformed to "Next".
To set to a new file representing the starting or phase compositions press the <F3> [INPUT] function key.

Using the Function Keys in INPUT-mode

F1: Help   - displays all specific options of the INFOREX system and

F2: Notes  - involves 5 pages with tables deciphering indices, search words and flags used in the database.
F3: Next   - saves the data input and goes to a new dataset.
F4: Edit   - permits marking and copying blocks of the strings selected. (see User's Manual).
F5: Write  - writes to a file on '\INFOREX\SAVE\' disk directory or prints on printer if type 'PRN' instead of a file name.

F9: Quit - same as ESC, quits the current operation.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 8

NOTE: <Shift-F3> - enables you to come back to the initial screen from any stage of execution of the V/E/I-mode procedures.

## SELECTING RUN CONDITIONS

The SRC-option is implemented to perform search-match operations through the database according to some "filters".

### Using the Function Keys in SRC-mode

F1: Help - same as in other MAIN MENU options.
F2: Notes - same as in other MAIN MENU options.
F3: Next_Box- go to another active box (system type, name of igneous rock, combination of volatiles, containers, etc.).
F4: fO2 - allows one to specify a range of REDOX-conditions.
F5: Search - starts the SEARCH through the database.
F9: Quit - same as ESC, quits the current operation.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 9

## SELECTING PHASE ASSEMBLAGE

### Using the Function Keys in SPA-mode (1st step, DATA FILTERING)

F1: Help - same as in other MAIN MENU options.
F2: Notes - same as in other MAIN MENU options.
F3: Window - go to another active box (window).
F4: On/Off - enables/disables flag "√" in front of a string addressed to Phase Assemblages or References.
F5: Exclude - deletes strings marked to disable.
F9: Phases - Go to 2nd step.

### Using the Function Keys in SPA-mode (2nd step, CHOOSING PHASES)

F1,F2: - same as in other MAIN MENU options.
F3-F8: - Don't use the keys! (see User's Manual for information).
F9: Quit - quits the operation and returns to Main Menu.

NOTE: Move the highlighted field to a phase field and press "ENTER".

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 10

## SYSTEM CONFIGURATION

This option allows the user to change or input new igneous rock or synthetic system indicators, mineral abbreviations, containers, etc.

WARNING! The use of SC-option requires an in-depth knowledge of INFOREX system. Read the User's Manual with attention!

### Using the Function Keys in SC-mode

F1: Help - same as in other MAIN MENU options.
F2: Notes - same as in other MAIN MENU options.
F3: Window - switches between windows (excepting for Buffers!).
F4: New - add a new Phase, System, Container or Settings file name.
F5: On/Off - enables/disables flag "√" in front of a string.
F6: Load - loads a file containing previously arranged settings.

F7: Save - saves current settings to a file.
F9: Quit - quits the operation and returns to Main Menu.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 11

EXCHANGE INFOREX DATA

Here you can:

- EXPORT all data linked with a reference to a separate file - just press <F2> key, then select a reference and type a file name to be created. The file exported is now ready to import, if you are going to send it to another user of INFOREX.

- IMPORT a data set directly to the INFOREX database - press <F3> key, select a file to be imported (".imp" extension!) and press "Enter".

NOTE: All strings in the imported files must be formatted exactly as described in the User's Manual: you will find there commentaries on all error messages.
One can UNDO the import operations IMMEDIATELY after a reference was imported - just press <F5> key as prompted at the bottom of EID-option screen (the undo procedure doesn't work if you have leaved the EID-option after import operations).

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 12

PETROLOGICAL CALCULATIONS

We have included in INFOREX few special functions which could be useful in petrological studies. Those can be called from MAIN MENU by pressing the <F7> key followed by selection of one of 5 function:

1. MINERAL-MELT GEOTHERMOMETERS: development of expressions describing mineral-melt equilibria in terms of temperature, pressure, fO2, and liquid (glass) composition.
2. Fe3+/Fe2+ RATIO CALCULATION: calculations of ferric-ferrous species in silicate melts as a function of temperature, fO2, and composition.
3. WATER SOLUBILITY: calculations of water contents in experimental glasses obtained in water-saturated conditions.
4. SPECIAL TOOLS: recast of experimental glass compositions to 100% with an ability to create files for testing COMAGMAT and METEOMOD models.
5. TERNARY DIAGRAMS: calculations of projection parameters for plotting experimental glass compositions onto ternary diagrams.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 13

Petrological Calculations: MINERAL-MELT GEOTHERMOMETERS

This option allows one to create a system of equations describing 1 atm pressure mineral-melt equilibria for OL, PL, AUG, PIG, OPX and SPINels. Following the extraction of a set of experimental data using INFOREX (including tables of coexisting mineral and glass compositions - F5 key) the calibration of the equations is accomplished by multiple regression in the form of a modified Arrhenius relation:

$$\ln K_i = A/T + B\log fO_2 + C \ln(Fe^{3+}/Fe^{2+})_L + D\ln RL + E,$$

where Ki is an equilibrium constant of a mineral-forming reaction, distribution coefficient or exchange constant for component-i, T is the absolute temperature, fO2 is oxygen fugacity, RL is a melt structure-chemical parameter, such as Si/O, NBO/T, Al/Si, (Na+K)/Al, etc., while the parameters A, B, C, D and E are the regression constants.
After the regression parameters are calculated, the option calculates

the statistics on goodness of fit, comparing the calculated and experimental values.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 14

Petrological Calculations: Fe3+/Fe2+ RATIO CALCULATION

1.Sack R.O.,Carmichael I.S.E.,Rivers M.,Ghiorso M.S.(1980) Ferric-ferrous equilibria in natural silicate liquids at 1 Bar. CMP 75: 369-376.
2.Kilinc A.,Carmichael I.S.E.,Rivers M.,Sack R.O.(1983) The Ferric-ferrous ratio of natural silicate liquids equilibrated in air. CMP 83: 136-140.
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4.Borisov A.A.&Shapkin A.I.(1990) A new empirical equation rating Fe3+/Fe2+ in magmas to their composition, oxygen fugacity, and temperature. Geochem. Intern. 27(1); 111-116.
5.Mysen B.O. (1991) Relations between structure, redox equilibria of iron, and properties of magmatic liquids.Physical Chemistry of Magmas. Advances in Physical Geochemistry. V. 9. New-York (Springer-Verlag): 41-98.
6.Kress V.C.&Carmichael I.S.E.(1991)The compressibility of silicate liquids containing Fe2O3 and the effect of composition,temperature,oxygen fugacity and pressure on their redox states. CMP 108: 82-92.
7.Nikolaev G.S., Borisov A.A., Ariskin A.A. (1996) Calculation of the Fe3+/Fe2+ ratio in magmatic melts: testing and additional calibration of empirical equations for various petrochemical series. Geochem. Intern. 34(8): 641-649.

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 15

Petrological Calculations: WATER SOLUBILITY

This option allows one to calculate water content in experimental glasses saturated with H2O and test experimental H2O contents at given conditions.

MODELS INVOLVED IN THE CONSIDERATION:

Burnham C.W. (1994) Development of the Burnham model for prediction of the H2O solubility in magmas. Volatiles in Magmas. Reviews in Mineralogy. V. 30: 123-129.
IMPORTANT: ONLY for basalts and andesites, not for granites and rhyolites!

Dixon J.E.,Stolper E.M.,Holloway J.R. An experimental study of water and carbon dioxide solubilities in mid-ocean ridge basaltic liquids. J. Petrol. in press.
ALGORITHM: Holloway & Blank (1994) Reviews in Miner. V. 30: 187-230.

Almeev R.R., Ariskin A.A. (1996) Mineral-melt equilibria in a hydrous basaltic system: computer modeling. Geochem. Intern. 34(7): 563-573.
EMPIRIC:lnC(H2O)=4.39+(48438*Si/O-14710)/T+0.59*lnP-21.45*Si/O+3.89*Al/Si

Esc - exit PgUp/PgDn

26 25

On-Line Help Facility 16

Petrological Calculations: SPECIAL TOOLS

This option allows one to recast INFOREX experimental glass compositions as a prelude for the further processing and graphic presentation:

FUNCTIONS AVAILABLE TO DATE:

1 Recast to 100 per cent including H2O as follows:
Σ=SiO2+..+H2O, SiO2'=100*(SiO2/Σ) etc
Name of output file: RECAST_1.DAT

2 Recast to 100 per cent excluding H2O (dry residue) as follows:
Σ=SiO2+..Cr2O3, SiO2'=100*(SiO2/Σ) etc
Name of output file: RECAST_2.DAT

3 Create file for testing the mineral-melt equilibrium temperatures to be calculated with COMAGMAT program (Ariskin et al.,1993):
Will be created from experimental glass compositions, including 12 major

```
   element contents with the value of experimental TEMP in the end of row.
   Name of output file: **_THERM.DAT

Esc - exit                                                          PgUp/PgDn
26 25
                    On-Line Help Facility                                  17
            Petrological Calculations: TERNARY DIAGRAMS

  The purpose of the function is to calculate parameters for projecting
experimental glass compositions onto ternary diagrams routinely used in
petrology. To use this function one should first create datafiles, like
OL_LQ.DAT, PL_LQ.DAT, etc. by means of SPA-option.

The list of ternary diagrams included is followed:
1. AB-AN-QTZ     (Tormey et al.,1987)  6. OLIV-DI-PLAG (Tormey et al.,1987)
2. AB-AN-CPX     (Tormey et al.,1987)  7. OLIV-CPX-QTZ (Walker et al.,1979)
3. PLAG-CPX-QTZ  (Tormey et al.,1987)  8. OLIV-PLAG-CPX(Walker et al.,1979)
4. OLIV-PLAG-QTZ(Tormey et al.,1987)  9. OLIV-PLAG-QTZ(Walker et al.,1979)
5. OLIV-DI-QTZ   (Tormey et al.,1987) 10. AFM, FeO/MgO, ALK, MG#, CA#, AL#

   Details of the calculations one can find in papers given in the window
called "FULL REFERENCE". The output files are saved in D:\INFOREX\SAVE\
directory. These files contain parameters necessary to put experimental
points onto ternary diagrams using any standard graphics package.
   The name of an output file includes first two letters to be the same as
in initial datafile, followed by _TRN plus the number of diagram in the
list above (e.g., OL_TRN_3 if OL_LQ.DAT was used an initial datafile).
Esc - exit                                                          PgUp
26 25
                    On-Line Help Facility                                  18

                      ADDITIONAL COMMENTS

Esc - exit                                                          PgUp
```

## INFOREX abbreviations (NOTES.TXT file)

```
21 38
                  IGNEOUS ROCK AND SYSTEM INDICATORS
 N (No volatiles)   /   V (with Volatiles)    /   F (Fluid saturated)   1
 - (undozed) / + (dozed with minor or major elements, crystals, etc.)
TERRA( )/LUNAR(L)/METEORitic(M)/PLANETary(P)-Martian,Venusian/SYNTHetic(S)
  1 Peridotite    -> PER  15 Basalt        -> BAS  29 Eucrite       -> EUC
  2 Pyroxenite    -> PXT  16 AlkalineBAS   -> ALB  30 Howardite     -> HOW
  3 Lherzolite    -> LHR  17 High-Al_BAS   -> HAB  31 Diogenite     -> DGN
  4 Harzburgite   -> HAR  18 Andesit.BAS   -> ANB  32 Shergottite   -> SNC
  5 Kimberlite    -> KIM  19 Andesite      -> AND  33 WIncAllende   -> WIA
  6 Picrite       -> PIC  20 Dacite        -> DAC  34 Chondrite     -> CHN
  7 Komatiite     -> KOM  21 Rhyolite      -> RHY  35 ANT_series    -> ANT
  8 MiAmRu-rock   -> MAR  22 Syenite       -> SYE  36 Green_glass   -> GGL
  9 Amphibolite   -> AMP  23 Trachyte      -> TRA  37 Pyrolite      -> PYR
 10 Eclogite      -> ECL  24 Diorite       -> DIO  38 Synthetic     -> SYN
```

| | | |
|---|---|---|
| 11 Melilitite -> MEL | 25 Granodior. -> GRD | 39 Aug_Minette -> MNT |
| 12 Nephelinite -> NEP | 26 Granite -> GRN | 40 Tonalite -> TON |
| 13 Norite -> NOR | 27 Gneiss -> GNE | 41 Charnockite -> CHA |
| 14 Boninite -> BON | 28 Sedimentary -> SED | 42 _____ -> ___ |

Esc - exit PgDn

7 66

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

| N | Phase | File | Index | N | Phase | File | Index |
|---|---|---|---|---|---|---|---|
| 1 | Glass(melt) | LIQ | LQ | 19 | AlkFeldspar | ALFS | AF |
| 2 | Plagioclase | PLAG | PL | 20 | Apatite | APAT | AP |
| 3 | Olivine | OLIV | OL | 21 | Armalcolite | ARM | AR |
| 4 | Augite+Di | AUG | AU | 22 | Carbonate | CARB | CB |
| 5 | Pigeonite | PIG | PG | 23 | Epidote | EPID | EP |
| 6 | Clino-Px(*) | CPX | CP | 24 | Alumina-sil | ALSI | AS |
| 7 | Ortho-Px | OPX | OP | 25 | Quartz | QUAR | QU |
| 8 | ProthoPx(*) | PRPX | PR | 26 | Perovskite | PERV | PV |
| 9 | Ilm-Hem_sol | ILM | IL | 27 | Ps-brookite | PSBR | PB |
| 10 | MagnUlv_sol | MAGN | MT | 28 | Sulfide | SULF | SF |
| 11 | Spinel | SPIN | SP | 29 | Ca-perovsk | CAPV | Pc |
| 12 | Garnet | GARN | GR | 30 | Mg-perovsk | MGPV | Pm |
| 13 | Nepheline | NEPH | NP | 31 | Tourmaline | TOUR | TU |
| 14 | Leucite | LEUC | LC | 32 | Corundum | CRND | CO |
| 15 | Melilite | MEL | ML | 33 | Zircon | ZRCN | ZR |
| 16 | Ortho-Amph | AMPH | AM | 34 | Monticellit | MONT | MO |
| 17 | Clino-Amph | HORN | HB | 35 | Rutile | RUT | RU |
| 18 | Mica_(*) | MICA | MI | 36 | Sphene | SPHE | SH |

* see additional comments * see additional comments

Esc - exit PgUp/PgDn

17 45

INDECIES OF CONTAINERS AND OXYGEN BUFFERS 3

| Containers | Index | Oxygen buffers | Index |
|---|---|---|---|
| 1 Pt_loops | PTL | Iron-wustite | IW |
| 2 Graphite_caps.le | GRA | Wustite-magnetite | WM |
| 3 Fe_(±Pt_sat)c.psules | FEC | Iron-magnetite | IM |
| 4 Mo_capsule psule | MOC | Magnetite-hematite | MH |
| 5 Pt-Ag_capsule psule | PTA | Quartz-Fayalite-Magn. | QFM |
| 6 Pt_capsule psule | PTC | Iron-quartz-fayalite | IQF |
| 7 Ag-Pd_capsule psule | AGP | Nickel -NiO | NNO |
| 8 Gold_capsule psule | AUC | Cobalt -CoO | CCO |
| 9 Iridium_loops | IRL | Mn3O4 -MnO | MMO |
| 10 Peridotite_cappsule | PER | Graphite-CO-CO2-O2 * | COC |
| 11 Al2O3_crucibles | COR | Graphite-CO-CO2-O2 ** | COC |
| 12 Rh_capsule psule | REC | Graphite-COH system | GRS |
| 13 Pt-Rh_capsule psule | PRH | Graphite-methane (ND) | GCH |
| 14 Au-Pd_capsule_psule | AUP | _____ | ___ |

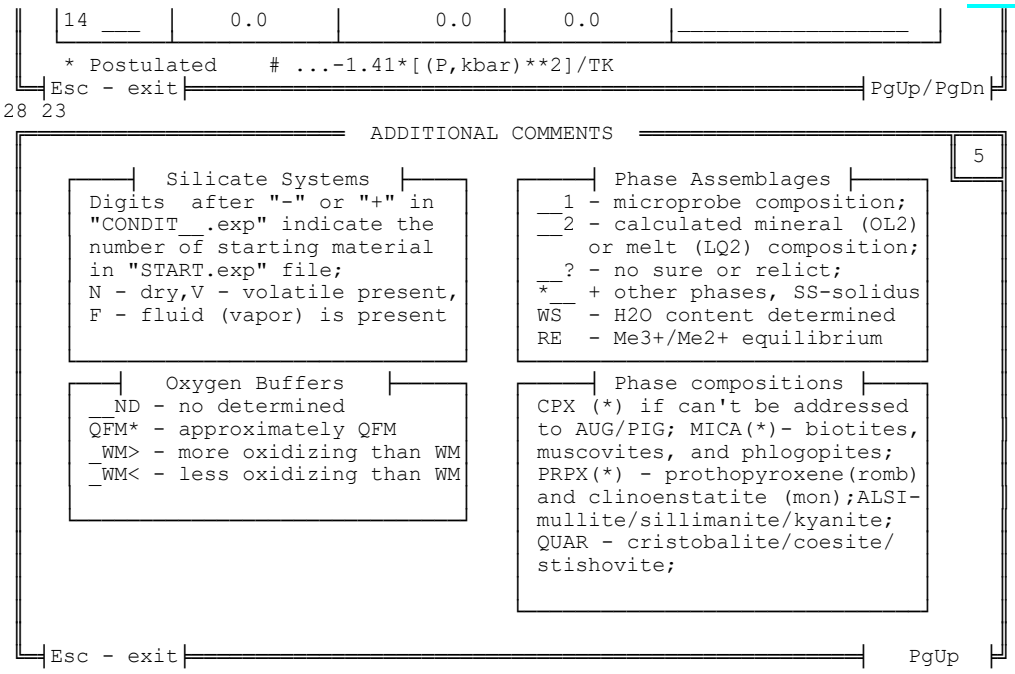
* >5 kbar, ** <5 kbar(see below)

Esc - exit PgUp/PgDn

24 32

PARAMETERS OF OXYGEN BUFFERS 4

| Buffer | lgfO2 = a0 + a1/TK + a2*(P,bar-1)/TK | | | References |
|---|---|---|---|---|
| | a0 | a1 | a2 | |
| 1 IW | 6.471 | -26834.7 | 0.055 | Myers,Eugster,1983 |
| 2 WM | 16.092 | -36951.3 | 0.083 | Myers,Eugster,1983 |
| 3 IM | 8.990 | -29260.0 | 0.061 | Huebner J.S.,1971 |
| 4 MH | 13.480 | -23847.6 | 0.019 | Myers,Eugster,1983 |
| 5 QFM | 8.290 | -24441.9 | 0.092 | Myers,Eugster,1983 |
| 6 IQF | 6.396 | -27517.5 | 0.050 | Myers,Eugster,1983 |
| 7 NNO | 9.360 | -24930.0 | 0.046 | Huebner, Sato, 1970 |
| 8 CCO | 7.936 | -25070.0 | 0.055 * | Myers,Gunter,1979 |
| 9 MMO | 13.380 | -25680.0 | 0.081 | Huebner, Sato, 1970 |
| 10 COC>5 | 2.740 | -19559.0 | 0.130 | Woermann et al.,1977 |
| 11 COC<5 | -0.044 | -20586.0 | -0.028 | French B.H., 1966 |
| 12 GRA | 4.620 | -22324.0 | 0.189 # | Ulmer, Luth, 1991 |
| 13 GCH | 0.0 | 0.0 | 0.0 | Eugster,Skippen,1967 |




# Appendix 2

## *List of INFOREX-4.0 (1997) experimental studies*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