Customer Support

Elsevier MDL offers a Helpdesk service to our customers. The Helpdesk will provide support for the use of the system and will answer questions you might have to other MDL products.

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Introduction
1 Introduction

This administrator’s guide explains and describes the installation, maintenance and settings files for both components of the CrossFire system:

The MDL CrossFire Commander (Client) and the MDL CrossFire Server

Starting with the MDL CrossFire Commander the setup processes on Windows platforms is described, followed by an explanation of the folder organization and the used files.

The section about the MDL CrossFire Server contains a description of the installation for both an update process and a complete new installation for the various platforms supported by the CrossFire system. It is followed by a description of the installation of the databases and their updates.

The appendix finally contains explanations of various topics, which are not covered by the other chapters.

The CrossFire team wishes you a trouble free installation and hopes that you enjoy the system.
The MDL CrossFire Commander
2 The MDL CrossFire Commander

MDL CrossFire Commander is the user interface to the MDL CrossFire Server system and the Databases CrossFire Beilstein and CrossFire Gmelin. It provides search functionalities that are dedicated to the structure of these databases and integrates them with other MDL content under DiscoveryGate.

The new MDL CrossFire Commander 7.0 provides all functionality for searching the databases and manage hitsets available in one Window.
Installation

2.1.1 GENERAL
This chapter describes the installation of the client software only. The setup can be stopped at any time by clicking the ‘Cancel’ button. You will also be able to navigate through the dialog boxes of the setup by using the ‘Next’ and ‘Back’ buttons until copying of the files will start.

It is recommended to close all programs that are currently running, even e-mail programs, before starting the installation.

The Windows Setup contains all necessary files for installing MDL CrossFire Commander under Windows NT4, Windows 2000 and Windows XP.

The Setup will copy all files into a target directory, which can be specified during the Setup process. The Setup will also ask for several parameters, which should be entered. Communication parameters, like MDL CrossFire Server address etc. can also be entered later from within the MDL CrossFire Commander Options menu (Define Server Profiles…).

Personal information like the license group name must be entered during the Setup. It will not be possible to skip the dialog for this information. Please ask your system administrator for details.

If the Setup has detected an old version of the MDL CrossFire Commander it extracts all necessary information for the use with the new version. You also have the option to keep a version of Commander V6 in parallel to the new one. This is for testing purposes only; the MDL CrossFire Structure Editor will not work properly for two versions of the Client Software. The MDL CrossFire Commander 7.0 CD also contains three additional products: Isis/Draw 2.5, LitLink and ChimePro 2.6 SP4. These Products can be installed by the setup as well.

Important Notes:

Help System

MDL CrossFire Commander 7.0 has a HTML based help system. Ensure that a Web browser is installed, which supports Java Script and that Java Script is enabled. Also ensure that the extension “*.htm” is connected with the desired Web browser. If MDL CrossFire Commander cannot find a Web browser or if other settings are wrong then an error message will appear. The help files are located in directory “Webhelp” under the MDL CrossFire Commander system directory.
2.1.2 THE INSTALLATION PROCESS

After inserting the MDL CrossFire Commander CD the following Dialog Box will appear:

Pressing “Install Commander” will start the setup process.
The following Dialog Box will appear either from InstallShell or by manually selecting the CrossFire Commander SETUP.EXE:

Press “Next” to begin the installation process…
Please read the license agreement. If you accept the license conditions you can proceed with “Next”…
This dialog box will appear only if MDL CrossFire Commander 7.0 setup has recognized an already existing MDL CrossFire Commander Installation.

You have the choice to either keep or remove this Installation (remove is recommended). Installing the new version in parallel should be done for testing purposes only.
Now you have the chance to choose your installation directory, default is c:\Program Files\MDL Crossfire Commander 7.0.
If MDL CrossFire Commander setup has recognized that communication parameter settings for the use with MDL CrossFire are missing, then it will ask you now for the missing parameters. If your are updating a previous installation this window will be skipped.
In the next step you will be asked about network parameters of the MDL CrossFire Server.

Please enter the IP Address or Hostname of your MDL CrossFire Server.
In this dialog box you have to enter your license group name. Contact your system administrator for this information. It is very important that a correct group name is entered here or you will not be able to use the CrossFire system. It is possible to change the group name three times after MDL CrossFire Commander is installed. This function is for emergency use only.
In this step you may select an additional structure editor for use with CrossFire Commander. The CrossFire Structure will be installed by default. If you need to install MDL Draw and MDL Isis Draw you may use the modify option after installing the first additional Structure Editor.
In this step you may for components to be used with Commander. Make sure, that no newer version of ChimePro will be overwritten.
Here you may configure/verify your LitLink access.
Installation Parameters Summary

Before the installation will start the setup will give you an overview on all parameters that have been entered so far.

At this point you have the chance to go back to change settings. If you click on 'Next' the installation will start.
A dialog boxes will show the proceeding of the installation.

Depending on whether you have selected additional components you will need to confirm their installation by pressing an OK button.
Finished

The final dialog box tells you whether the installation was succesfull or not. Click ‘Finish’ to complete the setup procedure.

After clicking the Finish button the installation is complete.

After a successful installation, you can start the Commander by either double-clicking the icon on your desktop or through the windows start menu.
2.2 Logon to the MDL CrossFire Server

After you have installed the MDL CrossFire Commander and entered all necessary information you may launch the MDL CrossFire Commander by double clicking the Commander icon. After the MDL CrossFire Commander has been started it will present a screen with buttons and windows. Please click on the button on the query Tab in order to establish a connection to the server.

If the Commander has all the necessary information it will present a login dialog box, prompting for your user id and the password.

![Server User ID and Password](image)

This information may be saved and you will not be prompted for this anymore.

If you recognize that the login does not proceed click the Close button and try to login again. If it still does not work, then please check your connection settings and group name and contact your system administrator.

After a successful logon on your CrossFire Server you will be present with the selection of available databases:
Please select one or more databases of your choice.
2.3 Start a search

After a query has been defined by using the query builder or with help of the predefined search forms you may click the Start Search button. A click on this button will send the displayed query with all its parameters to the MDL CrossFire Server and a search status report box will appear. This box includes a cancel button, which can be used to interrupt a search at any time. After the search has ended the status box will display whether your search had results or not. Pressing the view button will download your hits and display them on the results tab.
2.4 MDL CrossFire Commander Appendix

2.4.1 SYSTEM REQUIREMENTS (MINIMUM)

<table>
<thead>
<tr>
<th></th>
<th>IBM PC or compatible</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Platform</strong></td>
<td>Pentium Class PC</td>
</tr>
<tr>
<td><strong>Memory</strong></td>
<td>64 MB not including OS requirements and Help system requirements</td>
</tr>
<tr>
<td><strong>Storage</strong></td>
<td>70 MB hard disk storage</td>
</tr>
<tr>
<td><strong>Operating System</strong></td>
<td>MS Windows NT4 / 2000 / XP</td>
</tr>
<tr>
<td><strong>Protocol</strong></td>
<td>TCP/IP connection to server</td>
</tr>
</tbody>
</table>
2.4.2 NETWORK INSTALL OF THE MDL CROSSFIRE COMMANDER

The MDL CrossFire Commander can be installed on a network server into a write-protected directory. The system administrator has to start the Setup program and install the application into the desired drive/directory on the network. If a normal/restricted user wants to use this network installation several settings have to be made. Windows users should have a look at the logfile.txt, which is created during the Setup. It contains a description of all necessary operations. The MDL CrossFire Commander requires a XF.INI file, which has to be located in the MDL CrossFire Commander program directory. This file needs to contain the correct information about paths to users and group directories. Users must have write access to the users directories; group directories can be write-protected. Communication profiles, export settings and other settings can be made public for an entire user group in the group directory. Please refer to chapter “Files and Folders” for more details on the MDL CrossFire Commander directory structure.

The best method in a network environment is to copy all necessary setup files from the MDL CrossFire Commander CD-ROM onto a network drive and let the users install the MDL CrossFire Commander using the setup program.

2.4.3 PRECONFIGURED SETUP

If the system administrator prepares a XF.INI file and a DEFAULT.PRF file and copies them into the same directory where MDL CrossFire Commander 7.0 setup is located, then the setup program will use the information and install MDL CrossFire Commander 7.0 with the predefined settings without prompting the user for any additional information.

There are 2 types of the preconfigured setup:

1. Preconfigured Setup with a default.prf
2. Preconfigured Setup without a default.prf

In both cases a XF.INI file needs to be placed in the setup directory (with or without a default.prf)
If a default.prf exists, the hostname, username and password are taken from the default.prf. However if a host is specified in the xf.ini, this host is used instead.

A xf.ini file might look like this:

[XFCM]
ALERTS=NO
AUTONOM=NO
LITLINK=NO
LITLINK_FILTER=PY>"1970"
XFFE_ADDHELP1=Beilstein Reference Guide;50
XFFE_ADDHELP2=Gmelin Reference Guide;51
XFFE_ADDHELP3=AutoNom Help;52

[Install]
CrossFireGroup=default
GroupPath=d:\
WebHelpPath=d:\
FieldHelpPath=d:\
host=dbd-aix-ff2
## XF.INI keywords

<table>
<thead>
<tr>
<th>Section</th>
<th>Keyword</th>
<th>Content</th>
<th>Description</th>
</tr>
</thead>
</table>
| [XFCM]  | ALERTS     | YES or NO | YES: show Alerts tab in Commander  
NO: hide Alerts tab in Commander |
|         | AUTONOM    | YES or NO | YES: show Autonom tab in Commander  
NO: hide Autonom tab in Commander |
|         | LITLINK    | YES or NO | YES: show Litlink links in Commander  
NO: hide Litlink links in Commander  
Note: this setting can be changed by the user in the setup, depending if the user installs Litlink or not |
|         | LITLLINK_FILTER | PY>"yyyy" | Optional entry  
yyyy is a four digit year |
|         | XFFE_ADDHELPx | Desc, id | Defines the menu entries for additional help files in the Commander Help menu:  
x: 1, 2, 3 ...  
Desc: Description which will be displayed in the help menu  
id’s:  
- Beilstein: 50  
- Gmelin: 51  
- Autonom: 52  
- Patents: 53 |
<table>
<thead>
<tr>
<th>Section</th>
<th>Keyword</th>
<th>Content</th>
<th>Description</th>
</tr>
</thead>
</table>
| Install | CrossFireGroup     | Group   | Optional  
Group: the CrossFire Group. If no group is set, the user will be asked during the setup                                                |
| Host    | Host               | Host    | Optional  
If no host is defined the host from the default.prf will be used                                                                                 |
| GroupPath| Path               | Path    | Optional / The path to which the group folder will be copied. If this key does not exist, the default path will be used:  
“C:\Program Files\Mdl CrossFire Commander 7.0\group” |
| WebHelpPath | Path or URL     | Path    | Optional / Defines the location of the webhelp folder. This path must contain the “webhelp” folder.  
The default path of the WebHelp is:  
“C:\Program Files\MDL CrossFire Commander 7.0\WebHelp”. If this key is defined, the Setup will not install the WebHelp files in your installation path.  
It will change the path information in the local WebHelp index files: xfcm.hidx, xfsr.hidx and xfdh.hidx  
All WebHelp files may be copied to a network share or to a webserver. |
| FieldHelpPath | Path or URL   | Path    | Optional / Defines the location of the fieldhelp folder. This path must contain the “fieldhelp” folder.  
If a webhelp path is defined, the fieldhelp is not installed during the setup |
A default.prf might look like this:

default.prf:
HOST=direct.beilstein.com;
PORT=XFIRE8001;
UID=<XFUser>;
PWD=<XFUser>;
Password=<password>;

The keyword "Password=" will lock the profile so that nobody will be able to edit it. It is an ASCII file, of course, and everybody can open it with an Editor, but if one tries to open it with CrossFire Commander then it will be encrypted automatically.

The preconfigured setup works with both an ASCII “default.prf” and an encrypted file created or modified with Commander.

The easiest way of getting an XF.INI file and a DEFAULT.PRF is to copy them from an already existing installation of MDL CrossFire Commander and modify the XF.INI according to your needs.

Another interesting option is the combination of a preconfigured setup and the built-in features of Install Shell. You can easily prepare a preconfigured silent setup to install MDL CrossFire Commander. You just need to issue a preconfigured setup, while recording it with Install Shield.

Please refer to chapter 2.4.4 for further information.

2.4.4 SILENT INSTALLER / PUSH INSTALLER

The MDL CrossFire Commander Files can also be bundled into a self designed installer. Please refer to chapter 2.4.6 “Files and Folders”. For further information about this please refer to one of our MDL helpdesks.

You may also use the built-in capabilities of the install shell manufactured with InstallShield®.
2.4.4.1 Silent Install Overview

A regular (non-silent) setup receives the necessary input from the user in the form of responses to dialog boxes. However, a silent setup does not prompt the user for input. A silent setup must get its user input from a different source. That source is the Installation Shell Silent response file (.iss file). A response file contains information similar to that which an end user would enter as responses to dialog boxes when running a normal setup. Installation Shell Silent reads the necessary input from the response file at run time. The format of response files resembles that of an .ini file, but response files have .iss extensions. A response file is a plain text file consisting of sections containing data entries.

2.4.4.2 Recording a response file

You have the option of letting Installation Shell create the response file for you. Simply run your setup with the Setup.exe -r command line parameter. Installation Shell will record all your setup choices in Setup.iss and place the file in the Windows folder.

2.4.4.3 Play back the silent setup

After creating the response file, you are ready to run the setup in silent mode using Installation Shell Silent. When running a setup in silent mode, be aware that no messages are displayed. Instead, a log file named Setup.log captures setup information, including whether the setup was successful or not. You can review the log file and determine the result of the setup.

To launch Installation Shell Silent, run Setup.exe with the -s command line option. Installation Shell also provides the -f1 and -f2 switches so you can specify the name and location of the response file and the location of the log file. To verify if a silent setup succeeded, look at the ResultCode value in the [ResponseResult] section of Setup.log. Installation Shell writes an appropriate return value after the ResultCode keyname.

Please contact our helpdesk for further information.
2.4.5 MDL CROSSFIRE COMMANDER CONFIGURATION FILES

The MDL CrossFire Commander is using INI files for storing information on window sizes and last used files etc. The files XF.INI and XDK.INI are the most important INI files, because they contain essential information.

The file XF.INI must be located in the MDL CrossFire Commander program directory. It contains general information for the MDL CrossFire Commander system. The file XDK.INI is located in the users documents directory (e.g.: C:\Documents and Settings\"UserID\"\MDL\Commander\ini). Please refer to chapter “Files and Folder” for more details on the directory structure of a MDL CrossFire Commander 7.0 installation. The XDK.INI file must not be write protected. It contains user/workstation specific data.

If XF.INI and XDK.INI are missing MDL CrossFire Commander will not work correctly. All other INI files, which names start with "XF" (e.g. XFCM.INI) are not necessary and can be deleted if required. The system will then start with factory default settings. The XDK.INI file should at least contain the following lines (if c:\MDL CrossFire Commander 7.0 was selected as the installation destination directory):

Samples:

XF.INI
[XFCM]
ALERTS=YES
AUTONOM=YES
LITLINK=YES
SculptLauncher=HKEY_LOCAL_MACHINE\Software\InteractiveSimulations\Sculpt\Settings:SCULPT_LAUNCHER
Editor=ISISDraw
XFFE_ADDHELP1=Beilstein Reference Guide;50
XFFE_ADDHELP2=Gmelin Reference Guide;51
XFFE_ADDHELP4=AutoNom Help;52

36
[Install]
CrossFireGroup=<your group>
GroupPath=c:\group
UsersPath=c:\user

The keyword CrossFireGroup= must not be changed. If you need to change a group name then use the MDL CrossFire Commander Options menu for this purpose. It is possible to change the group name three times before you need to reinstall the software.

XDK.INI

[Install]
RootPath=ROOT
AvailablePorts=Xfire
ProfilePath=C:\DOCUMENTS AND SETTINGS\MDL\Commander\prf
StationID=HUA8MQII2…
StationName=malbus

[User]
DefaultProfile= default.prf
UserID=<XFUser>

This file is generated during the Setup process and will be adapted by MDL CrossFire Commander automatically if necessary.
### 2.4.6 FILE AND FOLDERS

#### 2.4.6.1 Folder Organisation of CrossFire Commander

During the installation, you will be asked for a target directory for the Commander. Below this target directory the setup will create a directory called "MDL CrossFire Commander 7.0", which will contain all binary files and DLLs together with the XF.INI file and the help management files *.HIDX. The default target directory for personal files is the My Documents folder.

The final directory structure will look like the following:

<table>
<thead>
<tr>
<th>1. General files</th>
<th>2. Personal files</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Diagram of general files]</td>
<td>![Diagram of personal files]</td>
</tr>
</tbody>
</table>

```plaintext
1. General files
   - MDL CrossFire Commander V7
     - fieldhelp
       - autonom
       - battlefield
       - gmelin
       - patients
     - group
       - dst
       - export
       - prf
       - samples
       - template
       - view
     - webhelp
       - autonom
       - battlefield
       - gmelin
       - patients
       - XTSR

2. Personal files
   - My Documents
     - MDL
       - Commander
         - dst
         - export
         - exportdate
         - history
         - ini
         - lgs
         - prf
         - queries
         - reports
         - view
```
**General Files:**

These folders will contain the following files:

**MDL CrossFire Commander 7.0:**

Binary files, DLLs, and XF.INI

**Fieldhelp:**

This directory contains various sub-directories with the HTML help system for MDL CrossFire Commander Fieldhelp.

**Group:**

This directory can be located elsewhere. It then has to be declared in the Commander Options Menu under Define Preferences. If Commander cannot find this directory then it will create it automatically in the XFC7 folder.

**group subfolders:**

**export:**

It is possible to create export settings files and export views. If you like to share them with a user group, simply copy all export files into this directory and the user group will have access to them.

**prf:**

It is possible to share communication profiles with a user group. Simply copy the profile file (extension *.prf) into this directory and all users will have access to this profile.

**template:**

This directory contains template files. These can be structure template files only but also query template files for the use in the Commander.

**view:**

It is possible to share user view definition files with a user group. Simply copy the user view files (extension *.udf) into this directory and all users will have access to this user view.

**Webhelp:**

This directory contains various sub-directories with the HTML help system for MDL CrossFire Commander.
Personal Files:

This directory can be located elsewhere. It then has to be declared in the Commander Options Menu under Define Preferences.

This directory must be write-able for the user. It is used by the Commander to store user defined files and settings. It is possible for a user to define his own export, communication and user view settings. They will be stored in this directory in the appropriate folders. Additionally this directory is used for storing personal INI files and the history. Therefore a new directory with the name of the current user will be created under this directory, which will then be used to store personal files in the appropriate directories as described above.

autonom:

This folder will be used by Commander to store BSD files, which will contain the history of a Autonom session. These BSD files can be opened with the Commander at any time using the File Open menu item.

dst:

Contains the datastructure files. After a connection to a CrossFire server has been established, Commander checks that both. Server and client, share the same DST files. If Commander recognizes that DST files are missing then it will start downloading them from the CrossFire server.

export:

This folder contains user defined export settings (extension *exs)

exportdata:

This folder contains executed and saved exports.

history:

This folder will be used by Commander to store BSD file, which will contain the history of a CrossFire session. These BSD files can be opened with the Commander at any time using the File Open menu item.

ini:

In this folder, Commander will store all INI files, which will be created during a session. The essential file in this directory is the XDK.INI file. If this file is deleted or corrupted then the Commander might not work correctly any longer. All other INI files can be deleted at any time. The Commander and its application will then start and run with factory settings.
logs:
This folder contains log files. Log files are produced e.g. for a query upload \textit{(execute query (List), execute query (SDF))}.

prf:
This folder contains server communication profiles (extension *.prf).

queries:
This folder contains saved user queries. They are shown in the My Queries node of the \textbf{Query Tab}.

reports:
This folder contains executed and saved reports.

view:
This folder contains user defined views (extension *udf)
2.4.6.2 Files of MDL CrossFire Commander

CrossFire Commander and its applications are using various files for storing information locally on the client side. If essential files are missing the Commander automatically tries to restore/create them. These essential files are: XF.INI, XDK.INI and the database DST files. In the following a description is given for these files.

2.4.6.2.1 INI Files

MDL CrossFire Commander uses the following INI files:

- **XF.INI**: Contains all settings of the Commander
- **XDK.INI**: XFDH.INI
- **XFSR.INI**: Contains all settings of the Structure Editor

2.4.6.2.2 BSD Files

These files contain structure, reaction or query definitions, which can be used by the Commander. They can be created using the File Save menu item of the Commander or the export function. They can be stored anywhere, but it is recommended to keep them together, in the users BSD folder.

2.4.6.2.3 BCCOM Files

These ASCII files are Commander command files used to perform a “Hop-Into” function. If they are opened with a double click (not edited with an ASCII/text editor) then the Commander will start automatically and will process the commands written in these files.

**Note:** MDL CrossFire Commander can also be run via command line either with the BCCOM file as parameter or with an @ symbol followed by a one line command.
General remarks:

Autostart settings in Commander will have priority over profile settings used in BCCOM files.

Keywords have to be entered in capital letters. The order doesn’t matter.

The file may contain any amount of line feeds.

The last character of the file must be a semicolon “;”

Syntax of BCCOM files:

“<name of the keyword>=<value>;;”

Keywords:

PROFILE (file name plus extension .prf. This keyword is optional)

DATABASE (either exact name or parts of it, e.g. BS or GM)

CONTEXT (S=substance, C=citations, R=reactions)

VIEW (ALL, ID, HITONLY, USER. This keyword is optional)

FILTER (PRODUCTS, EDUTCTS, BOTH. This keyword is optional)

QUERY or UPLOAD (list of numbers, which can be separated by any character; the target depends on the selected context; it does not check for valid RNs: if a RN is not available then the previous will be duplicated)

Query possibilities:

Mol- or RXNfile: QUERY=@@<path\filename>;

Fact-query: “QUERY="<fact query like in MDL CrossFire Commander>”

Structure/Reaction-query: “QUERY=<bsd string>”

embedded Mol- or RXNfiles

First line: all keywords as described above up to QUERY=
Second line: MOLFILE=

Third line: the first line of the Mol-/RXNfile or a blank line

Fourth line to nth line: subsequent lines of Mol-/RXNfile

Last line: single semicolon on a line of its own

**Alternate (New) Syntax of BCCOM files:**

XML-like tags enclose section with the following content:

<table>
<thead>
<tr>
<th>Tag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>&lt;TASK&gt;</code> ... <code>&lt;/TASK&gt;</code></td>
<td>Section for one query to be executed. A BCCOM file may contain multiple sections, which are executed consecutively. This tag pair appears on the outmost level and encloses one or more of the succeeding tags or tag pairs.</td>
</tr>
<tr>
<td><code>&lt;COMMENT&gt;</code> ... <code>&lt;/COMMENT&gt;</code></td>
<td>Free text</td>
</tr>
<tr>
<td><code>&lt;PROFILE&gt;</code> ... <code>&lt;/PROFILE&gt;</code></td>
<td>Name of the profile (*.prf file) to connect to the Xfire Server. This has no effect if Commander is already running and connected.</td>
</tr>
<tr>
<td><code>&lt;DATABASE&gt;</code> ... <code>&lt;/DATABASE&gt;</code></td>
<td>Name of the database to address, or name mask like <code>prefix*suffix</code>. No case sensitivity. A database is selected as follows among the ones available on the Xfire server: Full name match unless it is a mask. For a mask, match prefix and suffix separately. If the database currently selected fulfills the match, it is addressed, otherwise the first match. Use the name as a prefix, i.e. compare on the shortest common length. Again, prefer to address the database currently selected, if possible. Match on the first two characters of the name.</td>
</tr>
<tr>
<td><code>&lt;CONTEXT&gt;</code> ... <code>&lt;/CONTEXT&gt;</code></td>
<td>Database section where the query is to run: S for substances, R for reactions, C for citations.</td>
</tr>
<tr>
<td>Tag</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td><code>&lt;QUERY&gt; ... &lt;/QUERY&gt;</code></td>
<td>Same possibilities as for the old format (see above). For embedded molfiles, the enclosing tags should be each on a line of its own.</td>
</tr>
<tr>
<td><code>&lt;QUERIES&gt; ... &lt;/QUERIES&gt;</code></td>
<td>Name of a file containing one or more queries. The result sets of each particular query are merged to give a result. 2 file types are possible: SD file containing Molfiles. ASCII file where each line is either a fact query or a BSD string, both in the same format as would be allowed between the <code>&lt;QUERY&gt; ... &lt;/QUERY&gt;</code> tags. Lines with different query types may be mixed.</td>
</tr>
<tr>
<td><code>&lt;QUERYOPTIONS&gt; ... &lt;/QUERYOPTIONS&gt;</code></td>
<td>Keyword parameters like KEY=value; or KEY=lower_limit:upper_limit; to impose restrictions on a structure or reaction search:</td>
</tr>
<tr>
<td>NATOM</td>
<td>Number of atoms</td>
</tr>
<tr>
<td>NCOMP</td>
<td>Number of contiguous fragments</td>
</tr>
<tr>
<td>NPOSC</td>
<td>Sum of all positive charges</td>
</tr>
<tr>
<td>NNEGC</td>
<td>Sum of all negative charges</td>
</tr>
<tr>
<td>NCHRG</td>
<td>Sum of all charges</td>
</tr>
<tr>
<td>NRADI</td>
<td>Number of all radical dots</td>
</tr>
<tr>
<td>EXACT</td>
<td>All bonds searched have to match exactly, i.e. with no aromaticity involved. Specify 1 to turn on.</td>
</tr>
<tr>
<td>FREES</td>
<td>Implicit free sites on all atoms</td>
</tr>
<tr>
<td>DIFFC</td>
<td>Different fragments in the query must map to different fragments in the hit</td>
</tr>
<tr>
<td>IST</td>
<td>An additional unstructured fragment is required (specify 1) or forbidden (specify 2)</td>
</tr>
<tr>
<td>MIRROR</td>
<td>Require (1) or forbid (2) that a hit is flagged as a racemic compound</td>
</tr>
<tr>
<td>EXTRA</td>
<td>Forbid (1) that a hit is containing rings, which are not mapped to the query</td>
</tr>
<tr>
<td>---------------</td>
<td>--------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>STEREO</td>
<td>Map stereocenters and stereobonds in the query exactly (specify 1) to the hit, or (specify 2) to either the hit or its mirror image.</td>
</tr>
<tr>
<td>TAUTO</td>
<td>Allow tautomeric hydrogen or charge shifts in the hit in multiple attempts to map it onto the query (specify 1)</td>
</tr>
<tr>
<td>NOISO</td>
<td>Forbid any isotopes in the hit (specify 1).</td>
</tr>
<tr>
<td>NOMAP</td>
<td>Ignore any reaction center mappings in the query (specify 1)</td>
</tr>
<tr>
<td>&lt;UPLOAD&gt; ... &lt;/UPLOAD&gt;</td>
<td>List of RNs (or ID numbers in the context selected) separated by any character</td>
</tr>
<tr>
<td>&lt;VIEW&gt; ... &lt;/VIEW&gt;</td>
<td>Same as for the old format</td>
</tr>
<tr>
<td>&lt;FILTER&gt; ... &lt;/FILTER&gt;</td>
<td>Same as for the old format</td>
</tr>
<tr>
<td>&lt;SAVE&gt; ... &lt;/SAVE&gt;</td>
<td>After query execution, the hitset is saved under the name specified here. Characters allowed are letters, digits, and underscores with a maximum length of 28.</td>
</tr>
<tr>
<td>&lt;OPEN/&gt;</td>
<td>When specified, a new window will be opened for the results of the query or upload</td>
</tr>
<tr>
<td>&lt;EXPORT&gt; ... &lt;/EXPORT&gt;</td>
<td>An export of the hits is started using the export setting specified (file name without a path with a .exs extension like e.g. export.exs). The range of hits being exported is taken from the most current values in the DisplayHits application</td>
</tr>
</tbody>
</table>
2.4.6.2.4 PRF Files

These files are encrypted communication profiles and will be generated using the Commander Options/Connections menu item. They can be stored either in the group folder or in the users folder. The Commander will list only those PRF files in the appropriate dialog box, which are stored in the PRF folders.

2.4.6.2.5 DST Files

DST files are ASCII files containing a description of the fields of a CrossFire database. They are essential for factual searching and display. If DST files are missing on the Commander side then no database will be visible in the database selection listbox. Please refer to the system administrators guide for more details on these files.

2.4.6.2.6 EXS Files

These files contain export settings information. They are usually stored in the export folders.

2.4.6.2.7 UDF Files

These files contain user view definitions and are usually stored in the view folders.

2.4.6.2.8 HIDX Files

HIDX files are stored in the same folder where the corresponding executables reside. They contain information where the application can find the HTML help files and the context sensitive help. The first line (usually it starts with a “0”) describes the path to the main contents help file. The other lines are context sensitive help file links. There are two HIDX files prepared for Commander:

- xfdh.hidx: help management file for CrossFire Commander
- xfsr.hidx: help management file for CrossFire Structure Editor

In addition there are database specific hidx files to manage the Fieldhelp.

- xfaeco.hidx: Beilstein database
- xfgmel.hidx: Gmelin database

2.4.6.2.9 XFQUE Files

These files contain structure, reaction or query definitions, which can be used by the Commander. They can be created using the File Save menu item of the Commander. They can be stored anywhere, but it is recommended to keep them together, in the users queries folder.
The MDL CrossFire Server

3
3 The MDL CrossFire Server

This chapter describes the installation and usage of the MDL CrossFire Server software and databases on various operating systems. Please refer to the Appendix 3.10 for details on system limits and requirements and additional information.

The MDL CrossFire Server software provides access to large chemical databases. It consists of a server program for database searches and retrieval and of several additional programs for database installation, customer database creation and maintenance.

The MDL CrossFire Server supports two types of databases:

- The Beilstein and Gmelin files (read only databases), in one of its periodically updated versions. Presently, these files offer substructure search facilities, and the display of chemical structures and their data.

- Customer databases (read-write databases): Customer structures may be either loaded into a customer database from input files, or individually entered by users of the CrossFire client software. The same (sub)-structure search and display features as for a Beilstein database are available.

Our CrossFire Server software is available for Windows Platforms, AIX and Solaris Operating Systems.
3.1 Installation of the MDL CrossFire Server

The CrossFire delivery package consists of a server software CD and database tape cartridges labeled as follows:

- MDL CrossFire Server
- CrossFire Beilstein and / or CrossFire Gmelin
3.1.1 INSTALLATION PROCEDURE IBM AIX: NEW INSTALLATION

3.1.1.1 Checklist AIX: First/New Installation

The following provides a comprehensive checklist for the installation of MDL CrossFire Server software and CrossFire databases. A detailed description of every step is given where applicable and necessary.

If you want to know more about all of the various options of the used maintenance tools XFMAINT and XFMANAG please refer to the appropriate chapters in this guide.

3.1.1.2 Checklist for user “root” (System Administrator)

Step 1. Create a Group “xfire”

Create a user group named “xfire”. All CrossFire users on your system must be members of that group.

☐ Done

Step 2. Create/assign a CrossFire administrator id (e.g. xfireadm)

Select one CrossFire user to be the CrossFire administrator. As indicated later, the final installation steps and all CrossFire maintenance should be done under the CrossFire administrator login ID. The CrossFire administrator is owner of all CrossFire files, but does not need any specific system administrator rights. For database loading purposes the administrator must have the right to create files larger than 1 Gb.

☐ Done

Step 3. Create/assign CrossFire user

Note: A CrossFire user is a normal user of the operating system and belongs to the CrossFire user group (usually “xfire”). The user has to be installed using normal operating system routines. You cannot use XFMAINT for the purpose to add users to the CrossFire system.

☐ Done
Step 4. Prepare filesystems for CrossFire software and databases

a. Software filesystem

Create a filesystem, which will be used as the CrossFire Root directory (usually /xfire) with a minimum size of 100 MB to accommodate the MDL CrossFire Server software. For each future CrossFire user, add additional 20 to 30 MB to allow storage of hitsets and temporary files. Assign the CrossFire administrator ID and the CrossFire group to be owner of this directory:

```bash
chown xfireadm:xfire /xfire
```

(“xfireadm” will be the CrossFire administrator and “/xfire” the CrossFire root directory)

*Note: The CrossFire system only accepts filesystem names written in lower letters. All filesystems containing capital letters in the name will be ignored.*

The system administrator should proceed with the following.

Mount the file system at a mount point “/xfire”. This name is later referred to as the “CrossFire root directory” (ROOT). A different name may be chosen. The CrossFire root directory is not required to be a subdirectory of “/”, but may be created in any other directory.

☐ Done

b. Database filesystem

Create a filesystem or several filesystems, which can be used for storing CrossFire database files. You may choose any name for this/these filesystems (recommendation: /xfire/db/beil01 to /xfire/db/beilxx for the Beilstein database filesystems). The Beilstein database requires approx. 49 Gb (with the update 1. quarter 2004); the Gmelin database needs approx. 9 Gb. The Beilstein database has an annual growth of approx. 2 Gb.

Assign the CrossFire administrator ID and the CrossFire group to be owner of the corresponding directories /xfire/db/beil01 to /xfire/db/beilxx:

```bash
cd /xfire/db
chown xfireadm:xfire *
chmod 750 *
```

(if “xfireadm” will be the CrossFire administrator and “/xfire” the CrossFire root directory)

The CrossFire administrator needs to have write access to these filesystems, the CrossFire group only read access.

*Note: The CrossFire system only accepts filesystem names written in lower letters. All filesystems containing capital letters in the name will be ignored.*

☐ Done

Step 5. Adapt the System Timeouts

Currently, if the connection of an XFIRE user terminates irregularly and that user tries to reconnect with a different IP address (i.e. newly assigned by a provider), this may fail since a hanging XFIRE process from the former session is still consuming a license. To stop such processes after a reasonable timeout, connections accepted on the XFIRE port are assigned the SO_KEEPALIVE socket option: after an idle time of 2 hours the TCP/IP protocol detects, if the connection is still alive.
A shorter timeout value can be established for the entire system with the following shell commands:

```
no -o tcp_keepidle=<idle time>
```

and

```
no -o tcp_keepintvl=<time between subsequent probes of the connection>
```

The time unit is half seconds, e.g. for <idle time>=240 (2 min) and for <probe time>=20.

☐ Done

**Step 6. Adapt the “services” file in /etc**

The root user has to enter the following line into the file „services“ located in the „/etc“ directory:

```
xfired          8003/tcp
```

This will define a TCP service that is needed internally by the CrossFire daemon. The number entered here (default: 8003) has to be entered in the file „xfired.cfg“ located in the sys directory of the CrossFire installation as well (see below).

To start the CrossFire daemon if the system needs to be rebooted it is recommended to create a ”rc“ file, which has to be located in the /etc directory of the server. This rc file (name it „rc.xfire“) should contain the following statements:

```

cd /xfire/sys    # please enter the CrossFire directory name
./xfired > /dev/null
```

The file needs to be an executable file and the name of this file needs to be entered in the „rc.tcpip“ file.

☐ Done

**Step 7. Insert software CD into CD drive**

Ensure that all settings are correct and that the CD drive is available.

☐ Done

**Step 8. Mount software CD as a CD-ROM file system**

choose for example /cdrom as mountpoint

☐ Done

**Step 9. Switch to the installation directory**

Installation directory on CD is: /<cdrom filesystem>/inst/aix

☐ Done
Step 10. Execute Installation

Run the Installation program xfsetup with the specified name of the CrossFire Admin, and the desired filesystem (here: /xfire) for the MDL CrossFire Server e.g.:

$ xfsetup xfireadm /xfire

☐ Done

Step 11. Start CrossFire daemon

The CrossFire daemon can now be launched by the administrator (please note that the daemon software needs to be started using the complete path):

# cd /xfire/sys  # use actual CrossFire root directory
# $PWD/xfired

On success the ps command will show a process with the program name „xfired“. If the start of the CrossFire daemon was unsuccessful a log file will be found in the CrossFire sys directory:

xfm*.log
or
xll*.log

The asterisk is a placeholder for the process ID number.

This procedure is valid if the CrossFire daemon is used with the default port numbers 8001 to 8004. In all other cases the file XFIRED.CFG needs to contain the actual port numbers:

[Manager]
Port=control port (def: 8004);

[CrossFire]
Port=CrossFire user Port (def: 8001);
RootPath=;

[Accounting]
Port=Port for accounting (def: 8002);

[Licensing]
Port=Internal Port (def: 8003);

The internal port number has to be the same port number, which has been entered in the file /etc/services – see above.

If another directory name for the CrossFire root directory has been used instead of the default „/xfire“ then this actual CrossFire root directory name has to be entered in section [CrossFire] at the keyword „RootPath=“.

Note: To stop the CrossFire daemon, you have the choice:
command „STOP CROSSFIRE“ (using XFMANAG (see below)) or command “kill -TERM Process number“ (system command).

☐ Done

➢ BASIC INSTALLATION FINISHED
3.1.1.3 Checklist for user “xfireadm” (CrossFire Administrator)

Step 1. Make license disk / file available

You should copy the license file from disk or an other directory
to the <CrossFire root>/sys directory
[system commands]
$ cd /xfire/sys
$ dosread -D /dev/fd0 rs6000.xfl rs6000.xfl

☐ Done

Step 2. Launch XFMANAG and install license

Licenses are installed or modified by the CrossFire administrator using the CrossFire control
client XFMANAG. License files have the extension „XFL“ and are delivered on diskette or via
email (example below: rs6000.xfl). They have to be transferred into the CrossFire sys directory.
If no disk drive is available then copy the license file using FTP in ASCII mode. (command
parameters are described in the table below)

[system commands]
$ xfmanag

(Note: if port numbers other than default setting have been used
then XFMANAG has to be called with the following parameters:
“xfmanag localhost <port No>”. XFMANAG expect to establish a
connection to the CrossFire system using the control port, which is
defined in the file XFIRED.CFG. Default: 8004)

[control client prompt]
@XFMANAGE>set lic /localfile=rs6000.xfl

[. . . system messages]
@XFMANAGE>refresh lic
@XFMANAGE>set dump on
@XFMANAGE>set dump off
@XFMANAGE>quit

The commands „set dump on“ and „set dump off“ will create a complete XFIRED.CFG file,
which is used by the CrossFire daemon.

☐ Done

➢ SOFTWARE INSTALLATION FINISHED
**Install a database**

(Ensure that you have the rights to install files larger than 1 Gb!)

---

**Step 3. Execute XFMAINT in directory `<CrossFire root>/sys`**

☐ Done

---

**Step 4. Use Menu 1 to specify the location of database files (add filesystems)**

To accommodate Beilstein database files, your system administrator has created and mounted filesystems of a size that fits the size of the Beilstein Database (see above). Please refer to the filelist paper delivered with the tapes for details on the necessary size.

NOTE: XFMAINT is able to handle filesystems larger than 2 Gb.

Now XFMAINT needs to know which filesystems to use in order to calculate the necessary disk space and where to store the database files. This is done using menu 1. If menu 1 is selected you will see first an empty table of the file systems already defined to CrossFire and a prompt either to add or to remove a file system.

For each file system to be added, select option ‘a’ and enter the number of the file system name out of a displayed list of available file systems when prompted. Those file systems have to be provided by the root user.

**NOTE: XFMAINT can only work with filesystems which have names written in small letters and which are no links. XFMAINT is using the system command “df” for getting the necessary information. If you recognize that XFMAINT gets wrong results, then you may write a modified “df” and put it into the CrossFire sys directory. XFMAINT will then use the modified df.**

After this, return to the main menu by selecting ‘e’.

☐ Done

---

**Step 5. Database tape in tape drive**

Ensure that the first database tape is available in the tape drive and that the tape drive has got the correct settings (DLT requires a block size of “0”). You have to make the Tape drive available as root.

☐ Done
Step 6. Use Menu 2 to install the database

This will present an output, which may look like the following:

```
select: 2
No.  NAME        FILES      SIZE    ACCESS (R: read, A: r/w, N: disabled)
enter i (install from tape), r# (remove No. #), b# (backup No. #),
h (help), or e (exit).
select:

You will be prompted for various options. Select “i” for “installing from tape”. After this you are
prompted for the following information:

input file name: name of your tape drive (e.g. /dev/rmt#). The default is /dev/rmt0.
restore software or database: enter ‘d’.
continue: enter ‘y’ after inserting data tape cartridge No. 1.

At that point the maintenance program will load a list of all database files from tape. In case of
a reinstallation, an old filelist already may be present. Answer ‘n’ to the question to reuse it.
Based on the installation file list, xfmaint writes a shell script to the sys subdirectory of the
CrossFire root directory.

<CrossFire root>/sys/load.bat

Script generation will fail if insufficient space is available from file systems. Attempt to increase
space using menu 1.
If there is no need to modify (e.g. to use a tape changer) the script, you should choose to run it from xfmaint.
The copy process will take an estimated 10 hours for the Beilstein file in case of DLT IV or
about 2 hours in case of SDLT I tapes. The script will issue prompts and wait for insertion of
new tape cartridges.
If you are using a tape changer, you will have to edit the load.bat file appropriately, i.e. delete
all prompt commands and insert commands that will unload the cartridge (e.g. tctl offline and sleep 60)

☐ Done
Step 7. Check database with menu 7, 8 and 9

A database installation can be checked with the menu options 7, 8 and 9 in XFMAINT. Errors will be marked with "***" and stored in file "verify.err". With option 9 you can run MD5 checksum tests of your database files against a checksum file. Errors will be reported while the checksums will be written to a file "DBName.chk" in the sys directory. Depending on the errors you either might have to re-run the installation process, if some database files are missing, or you have to change the access rights. If you have to re-run the database installation then you need to go back to Step 6. and XFMAINT will produce a load.bat script, which will only load the missing files from tapes, not all of them.

☐ Done

Step 8. No errors: enable database with menu 4

If no errors have been found using menu options 7, 8 and/or 9 you need to select option No. 4 to enable the database. You should see a table (for the correct entries refer to the file list documentation) like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>N</td>
</tr>
</tbody>
</table>

The table shows the delivery of the Beilstein or other CrossFire database with the indicated number of bytes and files. The database is currently disabled (column ACCESS: N = no access).

To switch to the enabled state, enter “a1” (or more generally “a#” where # is the database number). The “access = N” column should change to “R” indicating that the Beilstein database is read-only, i.e. not modifiable by CrossFire Client users.

During the activation process you will be asked whether the database has been updated or not. If it is the first time you install this update you should answer with yes. This will write a update timestamp into the alert.cfg, the alert system will now recognize, that this database has been updated.

An Image with often used data will be created, this Image will be loaded into memory upon start of crossfire.

After being enabled, the CrossFire database is fully accessible to any user who is a member of the xfire group.

☐ Done

> DATABASE INSTALLATION FINISHED
**Step 9. Test system with MDL CrossFire Commander**

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

➢ CrossFire System Installed
3.1.2 INSTALLATION PROCEDURE IBM AIX: UPDATE

3.1.2.1 Checklist AIX: Update Software

In general the installation of a software update follows the above given procedure for installing the software. The whole update must be done as system administrator, root.

It is not possible to run CrossFire daemons of different versions in parallel. Therefore an old software installation needs to be replaced/overwritten. However, the new update will use the same settings as the old version.

The basic settings, like installing users and filesystems and tape drives, should have been done already. Therefore this chapter only presents a short checklist for installing the update. Please refer to the previous chapter if you need to know more details on specific tasks.

All MDL CrossFire Server settings will remain unchanged, since xfire.ini and xfired.cfg will not be overwritten.

Step 1. Stop CrossFire daemon

You can either stop the CrossFire daemon using the program XFMANAG (command: stop CrossFire) or by terminating the running daemon process (use the command “kill –term <process number>”).

☐ Done

Step 2. Security copy of XFLOG

If you are using a proprietary XFLOG program you should make a security copy of it now, because it will be overwritten with a new version provided by Elsevier MDL. If you are using the default program then you should skip this step.

☐ Done

Step 3. Insert software CD into CD drive

Ensure that all settings are correct and that the CD drive is available.

☐ Done

Step 4. Mount software CD as a CD-ROM file system

Choose for example /cdrom as mountpoint

☐ Done
Step 5. Switch to the installation directory

Installation directory on CD is: /<cdrom filesystem>/inst/aix

☐ Done

Step 6. Execute Installation

Run the Installation program xfsetup with the specified name of the CrossFire Admin and the desired filesystem (here: /xfire) for the MDL CrossFire Server e. g.:

$ xfsetup xfireadm /xfire

☐ Done

Step 7. Start CrossFire daemon

The CrossFire daemon can now be re-launched (please note that the daemon software needs to be started using the complete path):

$ cd /xfire/sys  # use actual CrossFire root directory
$ $PWD/xfired

On success the ps command will show a process with the program name „xfired“. If the start of the CrossFire daemon was unsuccessful a log file will be found in the CrossFire sys directory

☐ Done

Step 8. Create Database Image

Starting with CrossFire Server 7.0 some database files will be loaded into Memory upon start of CrossFire. This information will be compiled and written into an Image located in /xfire/bin/image.ini. If you install a new version of the CrossFire you need to rebuild this image, a new image will also be automatically created upon enabling or disabling of a database

☐ Done

Step 9. Test system with MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

➢ CrossFire System Installed
3.1.2.2 Checklist AIX: Update Database / Full Update

Depending on the amount of disk space that you have available for database files you also can install the database update in parallel to an existing database. You can keep the old database until the new database is installed and tested.

**Step 1. Insert first database tape into tape drive**

Ensure that all settings are correct and that the tape drive is available.

Make the tape drive available as root

☐ Done

**Step 2. Execute XFMAINT in directory <CrossFire root>/sys**

☐ Done

**Step 3. Use Menu 4 to disable old database**

This will present an output, which may look like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GM040200</td>
<td>103</td>
<td>9666408465</td>
<td>R</td>
</tr>
<tr>
<td>2</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>R</td>
</tr>
</tbody>
</table>

Enter “d” and the number of the database you want to disable. This will ensure that no users will have access to the database. If you enter “d2” in the above given example you will recognize that the R (=Read access) in column “A” will change to N (=No access).

☐ Done

**Step 4. Use Menu 2 to remove old database**

This will present an output, which may look like the following:

```
select: 2
No.  NAME     FILES SIZE ACCESS(R: read, A: r/w, N: disabled)
1 GM040200 103 9666408465 R
2 BS040300 250 48988779773 N
```

Enter i (install from tape), r# (remove No. #), b# (backup No. #), h (help), or e (exit).

select:
Select “r#” for removing the old database with the appropriate number. This will delete the removed database out of the list and will create a script “del.bat” which can be executed from xfmaint or later (you will find it in /xfire/sys).

☐ Done

**Step 5. Use Menu 1 to check for available disk space**

This will present an output, which may look like the following:

CrossFire filesystems for database storage:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>SIZE(B)</th>
<th>FREE(B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>/xfire/db/beil01</td>
<td>4697620480</td>
<td>4697620480</td>
</tr>
</tbody>
</table>

TOTAL 4697620480, FREE 4697620480

enter a (add filesystem), r# (remove No. #), n# (rename No. #), h (help), or e (exit):

XFMAINT will use all presented filesystems in this list for storing database files. Check the available disk space for the presented file system. If you recognize that the new database installation requires more disk space, add additional filesystems to this list using option a. Ensure that you do not have the CrossFire software filesystem available in this list!

☐ Done

**Step 6. Use Menu 2 to install new database**

This will present an output, which may look like the following:

select: 2

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS (R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GM040200</td>
<td>103</td>
<td>9666408465</td>
<td>R</td>
</tr>
</tbody>
</table>

enter i (install from tape), r# (remove No. #), b# (backup No. #), h (help), or e (exit).

select:

You will be prompted for various options. Select “i” for “installing from tape”. After this you are prompted for the following information:

* input file name: name of your tape drive (e.g. /dev/rmt#). The default is /dev/rmt0.

* restore software or database: enter ‘d’.

* continue: enter ‘y’ after inserting data tape cartridge No. 1.

At that point the maintenance program will load a list of all database files from tape. In case of a reinstallation, an old filelist already may be present. Answer ‘n’ to the question to reuse it.

Based on the installation file list, xfmaint writes a shell script to the sys subdirectory of the CrossFire root directory.

<CrossSFire root>/sys/load.bat
Script generation will fail if insufficient space is available from file systems. Attempt to increase space using menu 1.

If there is no need to modify (e.g. to use a tape changer) the script, you should choose to run it from xfmaint.

The copy process will take an estimated 10 hours for the Beilstein file in case of DLT IV or about 2 hours in case of SDLT I tapes. The script will issue prompts and wait for insertion of new tape cartridges.

If you are using a tape changer, you will have to edit the load.bat file appropriately, i.e. delete all prompt commands and insert commands that will unload the cartridge (e.g. tctl offline and sleep 60)

☐ Done

Step 7. Check database with menu 7, 8 and 9

A database installation can be checked with the menu options 7, 8 and 9 in XFMAINT. Errors will be marked with "****" and stored in file “verify.err”. With option 9 you can run MDS checksum tests of your database files against a checksum file. Errors will be reported while the checksums will be written to a file “DBName.chk” in the sys directory. Depending on the errors you either might have to re-run the installation process, if some database files are missing, or you have to change the access rights. If you have to re-run the database installation then you need to go back to Step 6. and XFMAINT will produce a load.bat script, which will only load the missing files from tapes, not all of them.

☐ Done

Step 8. No errors: enable database with menu 4

If no errors have been found using menu options 7, 8 and/or 9 you need to select option No. 4 to enable the database. You should see a table (for the correct entries refer to the file list documentation) like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>N</td>
</tr>
</tbody>
</table>

The table shows the delivery of the Beilstein or other CrossFire database with the indicated number of bytes and files. The database is currently disabled (column ACCESS: N = no access).

To switch to the enabled state, enter “a1” (or more generally “a#” where # is the database number). The “access = N” column should change to “R” indicating that the Beilstein database is read-only, i.e. not modifiable by CrossFire Client users.

During the activation process you will be asked whether the database has been updated or not. If it is the first time you install this update you should answer with yes. This will write a update timestamp into the alert.cfg, the alert system will now recognize, that this database has been updated.

An Image with often used data will be created, this Image will be loaded into memory upon start of crossfire.

After being enabled, the CrossFire database is fully accessible to any user who is a member of the xfire group.

☐ Done
Step 9. Test system with MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

➢ New Database Installed
3.1.3 INSTALLATION PROCEDURE SUN SOLARIS: NEW INSTALLATION

3.1.3.1 Checklist Solaris: First/New Installation

The following provides a comprehensive checklist for the installation of MDL CrossFire Server software and CrossFire databases. A detailed description of every step is given where applicable and necessary.

If you want to know more about all of the various options of the used maintenance tools XFMAINT and XFMANAG please refer to the appropriate chapters in this guide.

3.1.3.2 Checklist for user “root” (System Administrator)

Step 1. Create a Group “xfire”

Create a user group named “xfire”. All CrossFire users on your system must be members of that group.

☐ Done

Step 2. Create/assigna CrossFire administrator id (e.g. xfireadm)

Select one CrossFire user to be the CrossFire administrator. As indicated later, the final installation steps and all CrossFire maintenance should be done under the CrossFire administrator login ID. The CrossFire administrator is owner of all CrossFire files, but does not need any specific system administrator rights. For database loading purposes the administrator must have the right to create files larger than 1 Gb.

☐ Done

Step 3. Create/assign CrossFire user

Note: A CrossFire user is a normal user of the operating system and belongs to the CrossFire user group (usually “xfire”). The user has to be installed using normal operating system routines. You cannot use XFMAINT for the purpose to add users to the CrossFire system.

☐ Done
Step 4. Prepare filesystems for CrossFire software and databases

a. Software filesystem
Create a filesystem, which will be used as the CrossFire Root directory (usually /xfire) with a minimum size of 100 MB to accommodate the MDL CrossFire Server software. For each future CrossFire user, add additional 20 to 30 MB to allow storage of hitsets and temporary files.
Assign the CrossFire administrator ID and the CrossFire group to be owner of this directory:

chown xfireadm:xfire /xfire

("xfireadm" will be the CrossFire administrator and "/xfire" the CrossFire root directory)
Note: The CrossFire system only accepts filesystem names written in lower letters. All filesystems containing capital letters in the name will be ignored.
The system administrator should proceed with the following.

Mount the file system at a mount point "/xfire". This name is later referred to as the “CrossFire root directory” (ROOT). A different name may be chosen. The CrossFire root directory is not required to be a subdirectory of "/", but may be created in any other directory.

☐ Done

b. Database filesystem
Create a filesystem or several filesystems, which can be used for storing CrossFire database files. You may choose any name for this/these filesystems (recommendation: /xfire/db/beil01 to /xfire/db/beilxx for the Beilstein database filesystems). The Beilstein database requires approx. 49 Gb (with the update 1. quarter 2004); the Gmelin database needs approx. 9 Gb. The Beilstein database has an annual growth of approx. 2 Gb.
Assign the CrossFire administrator ID and the CrossFire group to be owner of the corresponding directories /xfire/db/beil01 to /xfire/db/beilxx:

cd /xfire/db
chown xfireadm:xfire *
chmod 750 *

(if "xfireadm" will be the CrossFire administrator and "/xfire" the CrossFire root directory)
The CrossFire administrator needs to have write access to these filesystems, the CrossFire group only read access.

Note: The CrossFire system only accepts filesystem names written in lower letters. All filesystems containing capital letters in the name will be ignored.

☐ Done

Step 5. Adapt the “services” file in /etc
The root user has to enter the following line into the file „services“ located in the „/etc“ directory:

xfired 8003/tcp
This will define a TCP service that is needed internally by the CrossFire daemon. The number entered here (default: 8003) has to be entered in the file „xfired.cfg“ located in the sys directory of the CrossFire installation as well (see below).

☑ Done

**Step 6. Insert software CD into CD drive**
Ensure that all settings are correct and that the CD drive is available.

☑ Done

**Step 7. Mount software CD as a CD-ROM file system**
Usually the CD will be mounted automatically upon insertion of the CD

☑ Done

**Step 8. Switch to the installation directory**
Installation directory on CD is: /<cdrom filesystem>/inst/sun

☑ Done
Step 9. Execute Installation

Run the Installation program xfsetup with the specified name of the CrossFire Admin, and the desired filesystem (here: /xfire) for the MDL CrossFire Server e.g.:

$ xfsetup xfireadm /xfire

☐ Done

Step 10. Start CrossFire daemon

The CrossFire daemon can now be launched by the administrator (please note that the daemon software needs to be started using the complete path):

# cd /xfire/sys  # use actual CrossFire root directory
# $PWD/xfired

On success the ps command will show a process with the program name „xfired“. If the start of the CrossFire daemon was unsuccessful a log file will be found in the CrossFire sys directory:

xfm*.log
or
xll*.log

The asterisk is a placeholder for the process ID number.

This procedure is valid if the CrossFire daemon is used with the default port numbers 8001 to 8004. In all other cases the file XFIRED.CFG needs to contain the actual port numbers:

[Manager]
Port=control port (def: 8004);

[CrossFire]
Port=CrossFire user Port (def: 8001);
RootPath=;

[Accounting]
Port=Port for accounting (def: 8002);

[Licensing]
Port=Internal Port (def: 8003);

The internal port number has to be the same port number, which has been entered in the file /etc/services – see above.

If another directory name for the CrossFire root directory has been used instead of the default „/xfire“ then this actual CrossFire root directory name has to be entered in section [CrossFire] at the keyword „RootPath=“.

Note: To stop the CrossFire daemon, you have the choice:
command „STOP CROSSFIRE“ (using XFMANAG (see below)) or
command „kill -TERM Process number“ (system command).

☐ Done

➢ BASIC INSTALLATION FINISHED
3.1.3.3 Checklist for user “xfireadm” (CrossFire Administrator)

**Step 1. Make license disk / file available**

You should copy the license file from disk or another directory to the `<CrossFire root>/sys` directory.

☑ Done

**Step 2. Launch XFMANAG and install license**

Licenses are installed or modified by the CrossFire administrator using the CrossFire control client XFMANAG. License files have the extension `.XFL` and are delivered on diskette or via email. They have to be transferred into the CrossFire `sys` directory. If no disk drive is available then copy the license file using FTP in ASCII mode. (Command parameters are described in the table below)

```system commands
$ xfmanag
```

(Note: if port numbers other than default setting have been used then XFMANAG has to be called with the following parameters: `xfmanag localhost <port No>`). XFMANAG expects to establish a connection to the CrossFire system using the control port, which is defined in the file `XFIRED.CFG`. Default: 8004)

```control client prompt
@XFMANAGE>set lic /localfile=solaris-1.xfl
[... system messages]
@XFMANAGE>refresh lic
@XFMANAGE>set dump on
@XFMANAGE>set dump off
@XFMANAGE>quit
```

The commands „set dump on“ and „set dump off“ will create a complete `XFIRED.CFG` file, which is used by the CrossFire daemon.

☑ Done

➤ **SOFTWARE INSTALLATION FINISHED**
Install a database

Step 3. Execute XFMAINT in directory `<CrossFire root>/sys`

☐ Done

Step 4. Use Menu 1 to specify the location of database files (add filesystems)

To accommodate Beilstein database files, your system administrator has created and mounted filesystems of a size that fits the size of the Beilstein Database (see above). Please refer to the filelist paper delivered with the tapes for details on the necessary size.

Now XFMAINT needs to know which filesystems to use in order to calculate the necessary disk space and where to store the database files. This is done using menu 1. If menu 1. is selected you will see first an empty table of the file systems already defined to CrossFire and a prompt either to add or to remove a file system.

For each file system to be added, select option ‘a’ and enter the number of the file system name out of a displayed list of available file systems when prompted. Those file systems have to be provided by the root user.

NOTE: XFMAINT can only work with filesystems which have names written in small letters and which are no links. XFMAINT is using the system command “df” for getting the necessary information. If you recognize that XFMAINT gets wrong results, then you may write a modified “df” and put it into the CrossFire sys directory. XFMAINT will then use the modified df.

After this, return to the main menu by selecting ‘e’.

☐ Done

Step 5. Database tape in tape drive

Ensure that the first database tape is available in the tape drive and that the tape drive has got the correct settings. You have to make the Tape drive available as root.

☐ Done
**Step 6. Use Menu 2 to install the database**

This will present an output, which may look like the following:

```
select: 2
No. NAME FILES SIZE ACCESS(R: read, A: r/w, N: disabled)
enter i (install from tape), r# (remove No. #), b# (backup No. #),
h (help), or e (exit).
select:
```

You will be prompted for various options. Select “i” for “installing from tape”. After this you are prompted for the following information:

- **input file name**: name of your tape drive (e.g. /dev/rmt#). The default is /dev/rmt0.
- **restore software or database**: enter ‘d’.
- **continue**: enter ‘y’ after inserting data tape cartridge No. 1.

At that point the maintenance program will load a list of all database files from tape. In case of a reinstallation, an old filelist already may be present. Answer ‘n’ to the question to reuse it.

Based on the installation file list, xfmaint writes a shell script to the sys subdirectory of the CrossFire root directory.

```
<CrossSFire root>/sys/load.bat
```

Script generation will fail if insufficient space is available from file systems. Attempt to increase space using menu 1.

If there is no need to modify (e.g. to use a tape changer) the script, you should choose to run it from xfmaint.

The copy process will take an estimated 10 hours for the Beilstein file in case of DLT IV or about 2 hours in case of SDLT I tapes. The script will issue prompts and wait for insertion of new tape cartridges.

If you are using a tape changer, you will have to edit the load.bat file appropriately, i.e. delete all prompt commands and insert commands that will unload the cartridge (e.g. `tctl offline and sleep 60`)

Done
Step 7. Check database with menu 7, 8 and 9

A database installation can be checked with the menu options 7, 8 and 9 in XFMAINT. Errors will be marked with "***" and stored in file "verify.err". With option 9 you can run MD5 checksum tests of your database files against a checksum file. Errors will be reported while the checksums will be written to a file “DBName”.chk in the sys directory. Depending on the errors you either might have to re-run the installation process, if some database files are missing, or you have to change the access rights. If you have to re-run the database installation then you need to go back to Step 6. and XFMAINT will produce a load.bat script, which will only load the missing files from tapes, not all of them.

☐ Done

Step 8. No errors: enable database with menu 4

If no errors have been found using menu options 7, 8 and/or 9 you need to select option No. 4 to enable the database. You should see a table (for the correct entries refer to the file list documentation) like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>N</td>
</tr>
</tbody>
</table>

The table shows the delivery of the Beilstein or other CrossFire database with the indicated number of bytes and files. The database is currently disabled (column ACCESS: N = no access).

To switch to the enabled state, enter “a1” (or more generally “a#” where # is the database number). The “access = N” column should change to “R” indicating that the Beilstein database is read-only, i.e. not modifiable by CrossFire Client users.

During the activation process you will be asked whether the database has been updated or not. If it is the first time you install this update you should answer with yes. This will write a update timestamp into the alert.cfg, the alert system will now recognize, that this database has been updated.

An Image with often used data will be created, this Image will be loaded into memory upon start of crossfire.

After being enabled, the CrossFire database is fully accessible to any user who is a member of the xfire group.

☐ Done

➢ DATABASE INSTALLATION FINISHED
Step 9. Test system with MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☑ Done

➢ CrossFire System Installed
3.1.4 INSTALLATION PROCEDURE SUN SOLARIS: UPDATE

3.1.4.1 Checklist Solaris: Update Software

In general the installation of a software update follows the above given procedure for installing the software. The whole update must be done as system administrator, root.

It is not possible to run CrossFire daemons of different versions in parallel. Therefore an old software installation needs to be replaced/overwritten. However, the new update will use the same settings as the old version.

The basic settings, like installing users and filesystems and tape drives, should have been done already. Therefore this chapter only presents a short checklist for installing the update. Please refer to the previous chapter if you need to know more details on specific tasks.

All MDL CrossFire Server settings will remain unchanged, since xfire.ini and xfired.cfg will not be overwritten.

Step 1. Stop CrossFire daemon

You can either stop the CrossFire daemon using the program XFMANAG (command: stop CrossFire) or by terminating the running daemon process (use the command “kill -term <process number>”).

☐ Done

Step 2. Security copy of XFLOG

If you are using a proprietary XFLOG program you should make a security copy of it now, because it will be overwritten with a new version provided by Elsevier MDL. If you are using the default program then you should skip this step.

☐ Done

Step 3. Insert software CD into CD drive

Ensure that all settings are correct and that the CD drive is available.

☐ Done

Step 4. Mount software CD as a CD-ROM file system

Usually the CD will be mounted automatically upon insertion.

☐ Done
Step 5. Switch to the installation directory

Installation directory on CD is: /<cdrom filesystem>/inst/aix

☐ Done

Step 6. Execute Installation

Run the Installation program xfsetup with the specified name of the CrossFire Admin and the desired filesystem (here: /xfire) for the MDL CrossFire Server e. g.:

$ xfsetup xfireadm /xfire

☐ Done

Step 7. Start CrossFire daemon

The CrossFire daemon can now be re-launched (please note that the daemon software needs to be started using the complete path):

$ cd /xfire/sys  # use actual CrossFire root directory
$ PWD/xfired

On success the ps command will show a process with the program name „xfired“.
If the start of the CrossFire daemon was unsuccessful a log file will be found in the CrossFire sys directory

☐ Done

Step 8. Create Database Image

Starting with CrossFire Server 7.0 some database files will be loaded into Memory upon start of CrossFire. This information will be compiled and written into an Image located in /xfire/bin/image.ini. If you install a new version of the CrossFire you need to rebuild this image, a new image will also be automatically created upon enabling or disabling of a database

☐ Done

Step 9. Test system with MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

➢ CrossFire System Installed
3.1.4.2 Checklist Solaris: Update Database / Full Update

Depending on the amount of disk space that you have available for database files you also can install the database update in parallel to an existing database. You can keep the old database until the new database is installed and tested.

**Step 1. Insert first database tape into tape drive**

Ensure that all settings are correct and that the tape drive is available.

Make the tape drive available as root

☐ Done

**Step 2. Execute XFMAINT in directory <CrossFire root>/sys**

☐ Done

**Step 3. Use Menu 4 to disable old database**

This will present an output, which may look like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GM040200</td>
<td>103</td>
<td>9666408465</td>
<td>R</td>
</tr>
<tr>
<td>2</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>R</td>
</tr>
</tbody>
</table>

Enter “d” and the number of the database you want to disable. This will ensure that no users will have access to the database. If you enter “d2” in the above given example you will recognize that the R (=Read access) in column “A” will change to N (=No access).

☐ Done

**Step 4. Use Menu 2 to remove old database**

This will present an output, which may look like the following:

```
select: 2
No.  NAME   FILES SIZE ACCESS(R: read, A: r/w, N: disabled)
1    GM040200 103  9666408465 R
2    BS040300 250  48988779773 N
```

enter i (install from tape), r# (remove No. #), b# (backup No. #), h (help), or e (exit).

select:
Select “#” for removing the old database with the appropriate number. This will delete the removed database out of the list and will create a script “del.bat” which can be executed from xfmaint or later (you will find it in /xfire/sys).

☐ Done

**Step 5. Use Menu 1 to check for available disk space**

This will present an output, which may look like the following:

CrossFire filesystems for database storage:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>SIZE(B)</th>
<th>FREE(B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>/xfire/db/beil01</td>
<td>4697620480</td>
<td>4697620480</td>
</tr>
</tbody>
</table>

TOTAL | 4697620480, FREE | 4697620480 |

enter a (add filesystem), r# (remove No. #), n# (rename No. #), h (help), or e (exit):

XFMAINT will use all presented filesystems in this list for storing database files. Check the available disk space for the presented filesystem. If you recognize that the new database installation requires more disk space, add additional filesystems to this list using option a. Ensure that you do not have the CrossFire software filesystem available in this list!

☐ Done

**Step 6. Use Menu 2 to install new database**

This will present an output, which may look like the following:

select: 2

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GM040200</td>
<td>103</td>
<td>9666408465</td>
<td>R</td>
</tr>
</tbody>
</table>

enter i (install from tape), r# (remove No. #), b# (backup No. #), h (help), or e (exit).

select:

You will be prompted for various options. Select “i” for “installing from tape”. After this you are prompted for the following information:

*input file name*: name of your tape drive (e.g. /dev/rmt0). The default is /dev/rmt0.
*restore software or database*: enter ‘d’. *continue*: enter ‘y’ after inserting data tape cartridge No. 1.

At that point the maintenance program will load a list of all database files from tape. In case of a reinstallation, an old filelist already may be present. Answer ‘n’ to the question to reuse it.

Based on the installation file list, xfmaint writes a shell script to the sys subdirectory of the CrossFire root directory.

<CrossFire root>/sys/load.bat
Script generation will fail if insufficient space is available from file systems. Attempt to increase space using menu 1.

If there is no need to modify (e.g. to use a tape changer) the script, you should choose to run it from xfmaint.

The copy process will take an estimated 10 hours for the Beilstein file in case of DLT IV or about 2 hours in case of SDLT I tapes. The script will issue prompts and wait for insertion of new tape cartridges.

If you are using a tape changer, you will have to edit the load.bat file appropriately, i.e. delete all prompt commands and insert commands that will unload the cartridge (e.g. tctl offline and sleep 60).

☐ Done

Step 7. Check database with menu 7, 8 and 9

A database installation can be checked with the menu options 7,8 and 9 in XFMAINT. Errors will be marked with "***" and stored in file "verify.err". With option 9 you can run MD5 checksum tests of your database files against a checksum file. Errors will be reported while the checksums will be written to a file "DBName.chk" in the sys directory. Depending on the errors you either might have to re-run the installation process, if some database files are missing, or you have to change the access rights. If you have to re-run the database installation then you need to go back to Step 6. and XFMAINT will produce a load.bat script, which will only load the missing files from tapes, not all of them.

☐ Done

Step 8. No errors: enable database with menu 4

If no errors have been found using menu options 7, 8 and/or 9 you need to select option No. 4 to enable the database. You should see a table (for the correct entries refer to the file list documentation) like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS (R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>N</td>
</tr>
</tbody>
</table>

The table shows the delivery of the Beilstein or other CrossFire database with the indicated number of bytes and files. The database is currently disabled (column ACCESS: N = no access).

To switch to the enabled state, enter “a1” (or more generally “a#” where # is the database number). The “access = N” column should change to “R” indicating that the Beilstein database is read-only, i.e. not modifiable by CrossFire Client users.

During the activation process you will be asked whether the database has been updated or not. If it is the first time you install this update you should answer with yes. This will write a update timestamp into the alert.cfg, the alert system will now recognize, that this database has been updated.

An Image with often used data will be created, this Image will be loaded into memory upon start of crossfire.

After being enabled, the CrossFire database is fully accessible to any user who is a member of the xfire group.

☐ Done
**Step 9. Test system with MDL CrossFire Commander**

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query "mp=100" in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

➢ New Database Installed
3.1.5 INSTALLATION PROCEDURE MICROSOFT WINDOWS NT / 2000 / 2003: NEW INSTALLATION

3.1.5.1 Checklist Windows Server Platforms: First / New Installation

The following provides a comprehensive checklist for the installation of MDL CrossFire Server software and CrossFire databases. This should help you with the installation, so that no step is overseen. A detailed description of the installation process is given where necessary.

The MDL CrossFire Server was developed under UNIX and was then ported to Microsoft’s Windows NT platform. Due to this fact, the MDL CrossFire Server sometimes requires commands in UNIX syntax that have to be interpreted using the program XFSCRIPT. But you will recognize that this is not a limitation.

If you want to know more about all of the various options of the used maintenance tools XFMAINT and XFMANAG then please refer to the appropriate chapters in this guide.

The CrossFire administrator must be member of the group “Administrators” to perform the following steps:

**Step 1. Create a local group “xfire” and edit Path variable**

Use the User Manager to create a local group xfire, which has to have the following rights:

- Log on as a service
- Log on locally

Every CrossFire user and the CrossFire administrator have to be members of this group.

*Note:* A CrossFire user is a normal user of the operating system and belongs to the CrossFire user group (usually “xfire”). The user has to be installed using normal operating system routines. You cannot use XFMAINT for the purpose to add users to the CrossFire system.

In addition the path variable needs to be modified to contain the CrossFire sys directory (e.g. d:\xfire\sys).

☐ Done

**Step2. Prepare hard disks for CrossFire software and databases**

*It is recommended* to use separate hard disks / volumes for MDL CrossFire Server and the databases. All hard disks have to be NTFS formatted for the use with CrossFire.

* a. hard disk / volume for software
The hard disk, which will contain the MDL CrossFire Server software, should have at least 2 Gb of free disk space available. This volume will be used to store not only static server software but also temporary user files, like hitsets or alerts.

☐ Done

b. hard disk / volume for database

Please refer to the filelist paper, which has been sent together with the database tapes, for more details on the necessary disk space you need to install the desired database. The Beilstein database requires approx. 49 Gb (with the update 1. quarter 2004); the Gmelin database needs approx. 9 Gb. The Beilstein database has an annual growth of approx. 2 Gb.

Ensure that the local group “xfire” has read access to this volume.

Note: If you want CrossFire to store database file not in the root directory of the desired volume but in a subdirectory of your choice, you need to prepare such subdirectories, assign the correct access rights and make them known to CrossFire using XFMAINT (see below).

☐ Done

Step 3. Adapt System Timeouts

Currently, if the connection of an XFIRE user terminates irregularly and that user tries to reconnect with a different IP address (i.e. newly assigned by a provider), this may fail since a hanging XFIRE process from the former session is still consuming a license. To stop such processes after a reasonable timeout, connections accepted on the XFIRE port are assigned the SO_KEEPALIVE socket option: after an idle time of 2 hours the TCP/IP protocol detects, if the connection is still alive. A shorter timeout value can be established for the entire system by inserting the following registry key:

HKEY_LOCAL_MACHINE\SYSTEM\CurrentControlSet\Services\Tcpip\Parameters\KeepAliveTime=...

The time value unit is milliseconds and you need to reboot your machine after this change. The probe interval has a reasonable default value.

☐ Done
Step 4. Adapt the “services” file

The administrator has to add the following line into the file

```
Drive: \Windir\system32\drivers\etc\services
```

(Drive and Windir are placeholders for the actual Windows NT / 2000 / 2003 system directory):

```
xfired 8003/tcp #xfired
```

Instead of “8003” any number can be used. This actual number has to be entered in the file XFIRED.CFG as well. After # you may add a comment.

☐ Done

Step 5. Connect a tape drive and make it available

Ensure that a DLT tape drive is installed and connected to the system.

Also ensure that any process, which might interfere with access to the tape drive (e.g. a backup), has been stopped for the time of the CrossFire database installation.

☐ Done

Step 6. Setup CD in CD ROM Drive and license disk / file available

☐ Done

Step 7. Switch to the installation directory

Installation directory on CD is <CDROM>:\inst\nti

☐ Done

Step 8. Execute Installation

Run the installation program xfsetup.bat with the specified destination directory for the MDL CrossFire Server e.g.:

```
z:\inst\nt>xfsetup d:\xfire
```

The batch file will create a directory d:\xfire and several subdirectories. It will assign the correct access rights and it will copy the initial MDL CrossFire Server files.

☐ Done
**Step 9. Start CrossFire service**

The administrator can use the following DOS command to start the CrossFire daemon:

d:\xfire\sys>d:\xfire\sys\xfired install

On success the Task Manager will show a process ‘xfired’.

This procedure is valid if the CrossFire daemon should be used with the default port numbers 8001 to 8004. In all other cases the file XFIRED.CFG needs to contain the actual port numbers:

```plaintext
[Manager]
Port=control port (def: 8004);

[CrossFire]
Port=CrossFire user Port (def: 8001);
RootPath=;

[Accounting]
Port=Port for accounting (def: 8002);

[Licensing]
Port=Internal Port (def: 8003);
```

- The internal port number has to be the same port number that has been entered in the file c:\winnt\system32\drivers\etc\services – see above.
- Under MS Windows NT based Operating Systems the CrossFire daemon will run as an installed service. This means that the daemon will be launched again, even if the system is rebooted.

The service can have the following attributes:

- Not installed.
- Installed, but not started.
- Started.

Installation and the start of the CrossFire daemon have to be done by an administrator.

If the start of the CrossFire daemon was unsuccessful a log file will be found in the CrossFire sys directory:

`xfm*.log`

or

`xll*.log`

The asterisk is a placeholder for the process ID number.

If the system will response with the following message

cannot create service:

`<error code>`

then CrossFire daemon may have been installed already, but not started. Try the following command first in order to remove the CrossFire daemon

```
d:\xfire\sys>d:\xfire\sys\xfired remove
```

and then try to start the service again. The latter command can also be used to stop the CrossFire system. The service can also be halted without removing it:

command „STOP CROSSFIRE“ under XFMANAG (see below)

Use the menu Start - Settings - Control Panel - Services (under NT 4.0) or Start – Programs – Administrative Tools – Services (under 2000) and you will get a list of all installed services. The CrossFire daemon has the name XFIRED and can be stopped and started at any time.
Step 10. License disk in disk drive and license file copied to <CrossFire root>\sys

Put the CrossFire license diskette into the floppy drive and copy the license file to the <CrossFire>\sys directory. License files have the extension "xfl".

☐ Done

Step 11. Launch XFMANAG and install license

Licenses are installed or modified by the CrossFire administrator using the CrossFire control client XFMANAG. Enter the following:

[System commands]
...>d:
d:/>cd \xfire\sys
d:\\xfire\sys>xfmanag
(Note: if port numbers other than the default settings have been used then XFMANAG has to be called with the following parameters: "xfmanag localhost <port No>"). XFMANAG expect to establish a connection to the CrossFire system using the licensing port, which is defined in the file XFIRED.CFG. Default: 8004)

[Control client prompt]
@XFMANAGE>set lic /localfile=nt.xfl

Several messages will be shown on the screen. If no error occurs then you will get the hint to use the command "refresh license" to activate the installed license.

[. . . system messages]
@XFMANAGE>refresh lic

This command will send a command to the CrossFire service and will activate the license. If you have got an error message in the step before please check the license file and contact Elsevier MDL.

The following commands will create a complete XFIRED.CFG file, which is used by the CrossFire daemon. If you will get the message “DENIED" you can ignore it at this stage.

@XFMANAGE>set dump on
@XFMANAGE>set dump off

Now the system is prepared for the installation of a database and you can exit XFMANAG using the command “quit”.

@XFMANAGE>quit

☐ Done

➢ SOFTWARE INSTALLATION FINISHED
Install a database

Step 12. Execute XFMAINT in directory <CrossFire root>\sys

Open an MS-DOS window and change to the directory "<CROSSFIRE root>\sys" (usually "d:\xfire\sys") and start the CrossFire maintenance program:

```
xfmaint <CROSSFIRE root> (e.g. "xfmaint d:xfire")
```

You will see a selection menu (please refer to the chapter “The CrossFire Maintenance Tool XFMAINT” for more details on this program).

☐ Done

Step 13. Use Menu 1 to specify the location of database files (add filesystems)

XFMAINT uses the term “filesystems” for identifying hard disks and subdirectories. At this stage XFMAINT needs to know where to store the database files. Menu 1 offers you the possibility to add hard disks and subdirectories to a list of known filesystems, which will be used by XFMAINT for calculating the necessary disk space and for creating a load.xfs for loading the database files from tape.

For each file system to be added, select option ‘a’ and enter the number of the hard disk out of a displayed list of available hard disks when prompted. It is recommended not to add the hard disk, which contains the MDL CrossFire Server software to this list.

If you want to force XFMAINT to produce a script file that will copy the database files into a specific subdirectory on the target drive, you have to rename the file system using menu option 1 after they have been added to the list. Enter the directory name together with the drive letter, e.g. “e:\bsdata” and NOT “bsdata” alone. Entering a subdirectory name without a drive letter will corrupt the XFIRE.INI file, which then has to be corrected manually.

After this, return to the main menu by selecting ‘e’.

☐ Done

Step 14. Database tape in tape drive

Ensure that the first database tape is available in the tape drive.

☐ Done
Step 15. Use Menu 2 to install the database

From the XFMAINT main menu select 2 to install the database. This will present an output, which may look like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>4898879773</td>
<td>N</td>
</tr>
</tbody>
</table>

enter i (install from tape), r# (remove No. #), b# (backup No. #), h (help), or e (exit).

select: i

You will be prompted for various options. Select “i” for “installing from tape”. After this you are prompted for the following information:

- enter input file name: name of your tape drive (e.g. \\TAPE0).
- enter blocking factor: 0 will accept any block size
- restore software or database: enter ‘d’.
- continue: enter ‘y’ after inserting the appropriate tape cartridge.

The database cartridges contain the database files. At that point the maintenance program will load a list of all database files from tape.

If you will get an error message at this point then most likely a wrong blocking factor has been used. Just retry it again using a different value.

If an old filelist file is already present in the sys directory then XFMAINT will prompt you for reusing it. Answer this prompt with ‘n’. Based on the installation file list, xfmaint writes a shell script called load.xfs to the sys subdirectory of the CROSSFIRE root directory. You can choose to run this script from within xfmaint.

You can also leave the xfmaint program and execute the script load.xfs using the program XFSCRIPT to complete the database installation.

d:\xfire\sys> xfscript load.xfs

The copy process will take an estimated 10 hours for the Beilstein file if you are using DLT IV tapes. The script will issue prompts and wait for insertion of new tape cartridges. If you are using a tape changer, you will have to edit the load.xfs file appropriately.

☐ Done
Step 16. Check database with menu 8 and 9

A database installation can be checked with the menu option 8 and 9 in XFMAINT. Errors will be marked with “***” and stored in file “verify.err”. Depending on the errors you either might have to re-run the installation process again, if some database files are missing, or you simply have to change the access rights. If you have to re-run the database installation again then you need to go back to Step 17, and XFMAINT will produce a load.xfs script which will only load the missing files from tapes.

☐ Done

Step 17. No errors: enable database with menu 4

If no errors have been found using menu options 7, 8 and/or 9 you need to select option No. 4 to enable the database. You should see a table (for the correct entries refer to the file list documentation) like the following:

```
No.  NAME        FILES      SIZE    ACCESS(R: read, A: r/w, N: disabled)
1    BS040300    250       48988779773 N
```

The table shows the delivery of the Beilstein or other CrossFire database with the indicated number of bytes and files. The database is currently disabled (column ACCESS: N = no access).

To switch to the enabled state, enter “a1” (or more generally “a#” where # is the database number). The “access = N” column should change to “R” indicating that the Beilstein database is read-only, i.e. not modifiable by CrossFire Client users.

After being enabled, the CrossFire database is fully accessible to any user who is a member of the xfire group.

☐ Done

DATABASE INSTALLATION FINISHED

Step 18. Test system with MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

CrossFire System Installed
3.1.6 INSTALLATION PROCEDURE MICROSOFT WINDOWS NT / 2000 / 2003: UPDATE

3.1.6.1 Checklist Windows Server Platforms: Update Software

In general the installation of a software update follows the above given procedure for installing the software.

It is not possible to run CrossFire daemons/services of different versions in parallel. Therefore an old software installation needs to be replaced/overwritten. However, the new update will use the same settings as the old version.

The basic settings, like installing users and filesystems and tape drives, should have been done already. Therefore this chapter only presents a short checklist for installing the update. Please refer to the previous chapter if you need to know more details on specific tasks. This procedure has to be performed as administrator.

Step 1. Stop CrossFire service

Ensure that no users are currently using the CrossFire system (command “users” in XFMANAG), open an MS-DOS window and switch to the CrossFire sys directory. Enter the following command at the DOS prompt:

```
xfired remove
```

This will remove the CrossFire service cleanly. It is also possible to stop the service using the Task Manager of Windows NT or to use the program XFMANAG (command: stop CrossFire).

☑ Done

Step 2. Security copy of XFLOG.EXE

If you are using a proprietary XFLOG.EXE program then you should make a security copy of it now, because it will be overwritten with a new version provided by Elsevier MDL. If you are using the default program then you can skip this step.

☑ Done

Step 3. Setup CD in CD ROM Drive and license disk / file available

☑ Done

Step 4. Switch to the installation directory

Installation directory on CD is <CDROM>:\inst\nti

☑ Done
Step 5. Execute Installation

Run the installation program xfsetup.bat with the specified destination directory for the MDL CrossFire Server e.g.:

```
z:\inst\nt>xfsetup d:\xfire
```

The batch file will install to the directory `d:\xfire` and several subdirectories. It will assign the correct access rights and it will copy the initial MDL CrossFire Server files. The setup will recognize a preexisting Server Installation and will preserve the existing xfire.ini and xfired.cfg, log files will not be removed.

☐ Done

---

Step 6. Start CrossFire service

The CrossFire service can now be re-launched using the following DOS command:

```
d:\xfire\sys>d:\xfire\sys\xfired install
```

On success the Task Manager will show a process „xfired“.

The CrossFire service should have used all previous settings and licenses and all databases should be available. You can check this using the program XFMANAG with the command “show license”.

☐ Done

---

Step 7. Create Database Image

Starting with CrossFire Server 7.0 some database files will be loaded into Memory upon start of CrossFire. This information will be compiled and written into an Image located in `/xfire/bin/image_ini`. If you install a new version of the CrossFire you need to rebuild this image, a new image will also be automatically created upon enabling or disabling of a database.

☐ Done

---

Step 8. Test system with MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

CrossFire System Installed
3.1.6.2 Checklist Windows Server Platforms: Update Database

In general the installation of a database update follows the above given procedure for installing the database.

The basic settings, like installing users and filesystems and tape drives, should be done already. Therefore this chapter only presents a short checklist for installing the update.

Depending on the amount of disk space that you have available for database files you also can install the database update in parallel to an existing database. Then you can wait removing the old database until the new database is installed and tested.

This procedure has to be performed as administrator.

Step 1. Insert first database tape into tape drive

Ensure that all settings are correct and that the tape drive is available.

☐ Done

Step 2. Execute XFMAINT in directory <CrossFire root>\sys

Open an MS-DOS window and change to the directory "<CROSSFIRE root>\sys" (usually "d:\xfire\sys") and start the CROSSFIRE maintenance program:

```
xfmaint <CROSSFIRE root> (e.g. “xfmaint d:\xfire”)
```

You will see a selection menu (please refer to chapter The CrossFire Maintenance Tool XFMAINT for more details on this program).

☐ Done

Step 3. Use Menu 4 to disable old database

This will present an output, which may look like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS(R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>GM040200</td>
<td>103</td>
<td>9666408465</td>
<td>R</td>
</tr>
<tr>
<td>2</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>R</td>
</tr>
</tbody>
</table>

Enter “d” and the number of the database you want to disable. This will ensure that no users will have access to the database. If you enter “d2” in the above given example you will recognize that the R (=Read access) in column “A” will change to N (=No access).
Step 4. Use Menu 2 to remove old database

This will present an output, which may look like the following:

```
select: 2
No. NAME        FILES      SIZE      ACCESS(R: read, A: r/w, N: disabled)
1   GM040200        103     9666408465 R
2   BS040300        250    4898879773 N
```

enter i (install from tape), r# (remove No. #), b# (backup No. #),
h (help), or e (exit).
select:

Select “#” for removing the old database with the appropriate number. This will delete the removed database out of the list and will create a script “del.bat” which can be executed from xfmaint or later (you will find it in /xfire/sys).

Step 5. Use Menu 1 to check for available disk space

This will present an output, which may look like the following:

```
CrossFire filesystems for database storage:
No. NAME                        SIZE(B)     FREE(B)
1   f:\bsdata\BS040300                   4697620480     4697620480
TOTAL   4697620480, FREE    4697620480
```

enter a (add filesystem), r# (remove No. #),
n# (rename No. #), h (help), or e (exit):

XFMAINT will use all presented filesystems in this list for storing database files. Check the available disk space for the presented file system. If you recognize that the new database installation requires more disk space, add additional filesystems to this list using option a. Ensure that you do not have the CrossFire software filesystem available in this list!

If you want XFMAINT to use a subdirectory on a given hard disk then you need to rename the filesystem with n#, where # represents the number of the filesystem in the list. Enter the directory name together with the drive letter, e.g. “f:\bsdata” and NOT “bsdata” without drive letter.

Ensure that you do not have the CrossFire software filesystem available in this list!

Exit this menu with “e”.

☐ Done
Step 6. Use Menu 2 to install new database

From the XFMAINT main menu select 2 to install the database. This will present an output, which may look like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS (R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>48988779773</td>
<td>N</td>
</tr>
</tbody>
</table>

Enter i (install from tape), r# (remove No. #), b# (backup No. #), h (help), or e (exit).

Select: i

You will be prompted for various options. Select "i" for “installing from tape”. After this you are prompted for the following information:

- enter input file name: name of your tape drive (e.g. \\TAPE0).
- enter blocking factor: 0 will accept any block size
- restore software or database: enter 'd'.
- continue: enter 'y' after inserting the appropriate tape cartridge.

The database cartridges contain the database files. At that point the maintenance program will load a list of all database files from tape.

If you will get an error message at this point then most likely a wrong blocking factor has been used. Just retry it again using a different value.

If an old filelist file is already present in the sys directory then XFMAINT will prompt you for reusing it. Answer this prompt with ‘n’. Based on the installation file list, xfmaint writes a shell script called load.xfs to the sys subdirectory of the CROSSFIRE root directory. You can choose to run this script from within xfmaint.

You can also leave the xfmaint program and execute the script load.xfs using the program XFSCRIPT to complete the database installation.

d:\xfire\sys> xfscript load.xfs

The copy process will take an estimated 10 hours for the Beilstein file if you are using DLT IV tapes or about 2 h in case of SDLT I tapes. The script will issue prompts and wait for insertion of new tape cartridges. If you are using a tape changer, you will have to edit the load.xfs file appropriately.

☐ Done

Step 7. Check database with menu 7, 8 and 9

A database installation can be checked with the menu options 7,8 and 9 in XFMAINT. Errors will be marked with "***" and stored in file “verify.err”. With option 9 you can run MD5 checksum tests of your database files against a checksum file. Errors will be reported while the checksums will be written to a file “DBName”.chk in the sys directory. Depending on the errors you either might have to re-run the installation process, if some database files are missing, or you have to change the access rights. If you have to re-run the database installation then you need to go back to Step 6. and XFMAINT will produce a load.bat script, which will only load the missing files from tapes, not all of them.

☐ Done
**Step 8. No errors: enable database with menu 4**

If no errors have been found using menu options 7, 8 and/or 9 you need to select option No. 4 to enable the database. You should see a table (for the correct entries refer to the file list documentation) like the following:

<table>
<thead>
<tr>
<th>No.</th>
<th>NAME</th>
<th>FILES</th>
<th>SIZE</th>
<th>ACCESS (R: read, A: r/w, N: disabled)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BS040300</td>
<td>250</td>
<td>4898779773</td>
<td>N</td>
</tr>
</tbody>
</table>

The table shows the delivery of the Beilstein or other CrossFire database with the indicated number of bytes and files. The database is currently disabled (column ACCESS: N = no access).

To switch to the enabled state, enter “a1” (or more generally “a#” where # is the database number). The “access = N” column should change to “R” indicating that the Beilstein database is read-only, i.e. not modifiable by CrossFire Client users.

After being enabled, the CrossFire database is fully accessible to any user who is a member of the xfir group.

☐ Done

**Step 9. Test system with MDL CrossFire Commander**

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Advanced Search Field. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and on the Result Tab you should be able to see a structure and the corresponding data.

In the options menu of the query tab you may use the entry “View Server Communication”. In the terminal view you will be able to see the actual communication between client and server. If an error occurred then this view will help you in identifying the underlying problem. If no error message occurs then CrossFire and the database have been installed successfully.

☐ Done

➢ New Database Installed
3.2 Validating the CrossFire Installation

There are two basic possibilities for checking a CrossFire installation: one for checking the correct installation of all database files and one for checking the CrossFire system itself. The first can be done using the program XFMAINT, which offers two menu options for this purpose. The second one can be done using the MDL CrossFire Commander.

3.2.1 DATABASE CHECKING USING XFMAINT

3.2.1.1 Menu Option 7: Verify Installation

XFMAINT will write a protocol file VERIFY.LOG for every session. This file can be viewed afterwards using any text editor. In addition XFMAINT will also create a file VERIFY.ERR, which contains error messages only.

Selecting menu option 7, you obtain a listing of all files known to all databases of a xfire root directory.

Apart from normal file information, the listing may contain messages starting with “***” and referring to the preceding file name. The problems they indicate may be fixed as follows:

- *** file inaccessible!
  The file cannot be accessed under the name printed. Possibly, it is stored in a different file system and should be moved, or it should be restored from a backup or installation tape.

- *** file mode should be ...
  The file should exhibit the indicated access mode for its owner (the xfire administrator), any xfire user, and other users (usually no access permitted). Change the file mode accordingly.

- *** file owner should be ........
  The xfire administrator should always be the owner, the group should read “xfire”.

- *** access control list should permit “rw-” to ...
  A xfire user enabled for updates to a customer database is permitted to update private files using an access control list.

- AIX: The “aclget” command should yield the following output for any private user file (as being listed in the verification output)

  attributes:
  base permissions
  owner(adm): rwx
  group(xfire): ---
others: ---
extended permissions enabled
permit rw- u:xfuser

where “adm” and “xfuser” are the login IDs of the administrator and the current user. If a different output is obtained, direct it to a file (say “fix”), edit it to contain the prescribed specifications, and apply it to the corresponding file using aclput "filename" < fix

• NT: with cacls you can check and modify permissions under NT based operating systems.

• *** error loading ...
  This message indicates a failure to access the configuration file of a specific user. Refer to the next chapter for more details and correction possibilities.

• *** file installed from tape: not found or incorrect size
  These messages indicate that a file specified in a tape file list <CROSSFIRE root>/sys/filelist (AIX) or <CROSSFIRE root>/sys/filelist (NT) cannot be found in its proper CROSSFIRE database or has a file size different from the value recorded in the file list (e.g. as result of a copy failure). You may delete an obsolete file list to further avoid the above messages.

3.2.1.2 Menu Option 8: Check File Readability

Selecting this menu option will first lead to the following request:

output to new log file (old: verify.001) ? [Y/(N)]:

If you answer with „Y“ the old verify file will be renamed and the result of the verification will be written in a new file VERIFY.LOG.

The next prompt will ask you for the database to check. Select the number together with the character „c“, e.g. c2.

XFMAINT will try to read 1 kb of every MB of a database file (small files will be read completely). If an error occurs on file open the process will be terminated. Otherwise it will give an error message (together with the position) and the check will continue.

This procedure may take a while, but ensures that all necessary files are readable.

You may interrupt the checking at any time by entering Ctrl-C (Break).

This option is faster than Option 9: a checksum verification, but checksums are more reliable.
### 3.2.1.3 Menu Option 9: Determine Checksums of Installed DBs

Selecting this menu option will first lead to the following request:

**output to new log file (old: verify.002) ? [Y/(N)]:**

If you answer with „Y“, the old verify file will be renamed and the result of the verification will be written in a new file VERIFY.LOG.

The next prompt will ask you for the database to check. Select the number together with the character „c“, e.g. c2.

XFMAINT will (after confirmation) start to create MD5 checksums for the database files defined in xfire.ini. If no checksum file for the selected database is available a warning will occur.

Note: creating MD5 checksums is very CPU intense and can last up to 2 hours in case of the Beilstein database.

### 3.2.2 System Check Using MDL CrossFire Commander

Checking all parts of the installation can be done best using the MDL CrossFire Commander. Run the client and try to establish a connection to the MDL CrossFire Server. If the connection can be made then you should get a database list showing the installed databases. Select one and enter the query “mp=100” in the Fact Query Window. Click the “Start Search” button. After a short time MDL CrossFire Commander should present a dialog box telling you that it has found hits. Click OK and Display Hits will get the focus and you should be able to see a structure and the corresponding data.

In the file menu of Display Hits you may use the entry “View Communication” to switch the Display Hits window to a terminal view, in which you will be able to see the actual communication between client and server. If an error had occurred then this view would help you in identifying the underlying problem. If no error message occurs then CrossFire and the database has been installed successfully.
3.3 The MDL CrossFire Server: Server Programs

3.3.1 THE CROSSFIRE MANAGER “XFIRED”

The CrossFire Manager or Daemon program is used for managing users and licenses. This program only runs once per physical server. It has to be started before the CrossFire system can be used and it needs to be active during the working time. Please refer to the chapter on the installation of the CrossFire software for details on settings for the CrossFire Daemon for a specific operating system.

3.3.2 THE MDL CROSSFIRE SERVER “XFIRE”

3.3.2.1 Line Mode Commands

The following descriptions and examples are done on an AIX system. The output may differ slightly on NT operating systems.

3.3.2.1.1 General Behavior

You may start the server in line mode by typing

```bash
xfire home <validgroupname>
```

in the /xfire/bin directory. After being invoked, the MDL CrossFire Server issues the following logo and prompts for the first command:

```
MDL CrossFire: Main Server Control Program.
MDL CrossFire Server Software, Version 7.0 (Build 23)
Copyright (c) MDL Information Systems GmbH 1996,2004

Usage: <program dir>/xfire <database> [root dir]

TIME = 60
HITS = 10000
SETS = 1
RUN at 000000
DATE = 20040223
MAIL = <yourmailserver>
FROM = <yourserveradmin@yourcompany.com>
PORT = 25
NUMA = 50
ALUS = 5
Last Update for BS: 20040204:071441
Last Update for PA: 20040220:132318
@XFMANAGE>
```

```bash
BIN: /xfire/bin/
SYS: /xfire/sys/
USR: /xfire/usr/
TMP: /xfire/tmp/
PRM:
Session timeout: 0 sec
```
Commands may be entered on single or multiple lines. Continuation of input is requested using a backslash before the carriage return or line feed. In this case, the server will re-issue the prompt to ask for the next line. Certain commands request additional input lines by specific "back prompts", see below. Command verbs may be abbreviated as long as they are unique, and are not case sensitive.

Output from a command is terminated by one of two prompts:

The @XFIRE> prompt will appear when all output is complete.

The SEND command may prompt back with a @NEXT> prompt if a limit on the number of output bytes has been specified. Expected input is <return> or n<return> to request continuation of output or b<return> to abort.

The server program is terminated using the EXIT command, Ctrl-D, or end-of-file when input is redirected from a file.

The response of the server to a command consists of formatted lines and message lines. Message lines are only for information and debugging purposes. Formatted lines provide the interpretable contents of the response and are the only ones considered by the CROSSFIRE client.

Formatted lines are introduced by two token characters:

// Data line. The line may be closed by the characters "@+". Data lines to a command are sent contiguously. The contents of data are obtained after stripping line termination characters (carriage return and line feed) and "//" plus "@+".

/M Hitset parameter line sent after completion of a search, or line with database limits returned in response to a corresponding information request.

/I Information message.

/U Message to be shown to the CROSSFIRE client user.

/W Warning message. The result of an operation may not be as expected.
/E  Error message. The command was not executed.

/F  Fatal error message. The server cannot operate due to an environment or installation error.
3.3.2.1.2 Command ADDCOMP

ADDCOMP <Customer RegNo>

The command adds a new entry to the customer database currently selected. As a response to the command line, the server prompts back using a @UP> prompt. The user should enter the data of a valid full structure or reaction as a data stream on multiple lines with all but the last line being terminated by backslash + <return>. For lines requesting continuation, the server issues further @UP> prompts and finally a @XFIRE> prompt.

The command succeeds if the following criteria are all met:

The current database is a properly installed customer database where the user has write access to the RegNo on the command.

The RegNo does not correspond to an existing entry.

The data stream entered is a valid representation of a full structure for a customer structure database, or a full reaction for a customer reaction database. Beyond being syntactically correct, it must not include structural query features.

Formats supported for structures are Rosdal or BSD (Beilstein Structural Data) for substances and BSD for reactions. Rosdal is described in a separate document, BSD, in chapter 4 of this paper.

Example: adding a reaction

@XFIRE>
addcomp 10020
@UP>
<BSD@<RXN@RID=103@DIRECTION=FORWARD@<STR@BRN=112@ROLE=EDUCT@ROSDAL=\ @UP>
(LF"C22H26O9S2",MO"16",CRN"103",ST2(8),ST1(11,12,14)) (SF"C22H26O9S2") 1S,\ @UP>
30, 40, 50, 8 (F0), 11 (F0), 12 (F0), 14 (F0), 150, 160, 190, 210, 240, 260, 270, 34H, 35H, \ @UP>
1-2, 1-3, 1=4, 1=5, 2=6, 2-7, 3=(A+) 8, 6-9, 7=10, 8-11, 8-12, 9=13, 10-13, 11-14, 11-1\ @UP>
5, 11-(A-) 35, 12-16, 12-(A-) 17, 13-18, 14-16, 14-19, 14-(A-) 34, 15-20, 17-21, 19-2\ @UP>
A1D1D3.@>STR@<STR@BRN=3137@ROLE=PRODUCT@ROSDAL=(LF"C8H16N2O3",MO"16",BRN\ @UP>
"3137",ST1(6,7,8,10)} (SF"C8H16N2O3") 1 (X55486, Y28592), 2O (X59118, Y25937), 3\ @UP>
O (X51853, Y25937), 4 (X52261, Y30758), 5 (X58320, Y30612), 6 (F0, X57734, Y21669), 7\ @UP>
(F0, X53238, Y21669), 8 (F0, X59118, Y17401), 9O (X51853, Y17401), 10 (F0, X55486, Y1\ @UP>
4746), 11N (X61969, Y16212), 12 (X55518, Y11065), 13N (X58515, Y9241), 14H (X49589,\ @UP>
Y21669), 15H (X60991, Y21669), 1-2, 1-3, 1-4, 1-5, 2-6, 3-7, 6-7, 6-8, 6-(A-) 15, 7-9, \ @UP>
3.3.2.1.3 Command CLEAR

The CLEAR command deletes all temporary hitsets of the current session. Temporary hitsets are distinguished by names starting with q or Q and otherwise consisting only of digits.

To also reset the automatic generation of temporary hitsets, it is necessary to switch to a different database (possibly HOME) and then to reselect the previous one.

Example:
@XFIRE>
clear
deleted: /usr/<xfireuser>/18590.2369966156/q01.hit
@XFIRE>
dbselect home
@XFIRE>
dbselect bs0304ae
/M MINSEQ=1, MAXSEQ=8861806, MINBRN=0, MAXBRN=9476792, UPDATES=0
@XFIRE>

3.3.2.1.4 Command DBDIR

Same command as DBLIST.

3.3.2.1.5 Command DBINFO

Textual information about the current database is returned.

Example:
@XFIRE>
dbinfo
// MDL CrossFire Server Software, Version 7.0 (Build 23)
// Copyright (c) MDL Information Systems GmbH 1996,2004
// Current database is 'BS0304AE' with 8861806 compounds.
// Beilstein Data: Copyright (c) 1988-2003, Beilstein Institut zur
// Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and
// MDL Information Systems GmbH. All rights reserved.
// Available contexts 'SRC' (Substances,Reactions,Citations).
// Current context 'S'.
// User 'xfireadm', rights 'R' (All,Read,None).
@XFIRE>
3.3.2.1.6 Command DBLIST

The command returns a data stream with keyword parameters about all databases available and their attributes:

```plaintext
@XFIRE>
dbdir
//RECLIENT=ON;REUSER=;DBNAMES=GM0302SF,GM0303SF,BSMINIAE,B0303AE,B0304@+
//AE,B030400AE,BSMINPR,B0303PR,B040300PR,BSMINIAB,B0303AB,B0304@+
//AB,B030400AB,B030400PA,DBTOKENS=GM0302SF,GM0303SF,BSMINIAE,B0303AE,B030@+
//04AE,B040300AE,BSMINPR,B0303PR,B040300PR,BSMINIAB,B0303AB,B0304@+
//04AB,B040300AB,PA030400PA;DBSYNTAX=1,1,1,1,1,1,1,1,1,1,1,1,1;DBACCESS@+
//R,R,R,R,R,R,R,R,R;DBMODE=ORG,ORG,ORG,ORG,ORG,ORG,ORG,ORG,ORG,ORG,ORG,ORG,ORG;CFDIR=xfgmel5.dst,xfgmel5@+
//dst,xfaeco5.dst,xfaeco7.dst,xfrea5.dst,xfrea7.dst,xfrea7.dst,xfabs5.dst,xfabs7.dst,xfabs7.dst,xfabs7.dst,xfabs7.dst,xfpat2@+
//.dst;CONTEXTS=SRC,0;SEARCHES=SRC,0;RECONNECT=15602_28802492;@+
@XFIRE>
```

The value to each keyword is a comma-separated list with the same number of entries.

Data available are explained in the following table:

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>DBNAMES</td>
<td>Names of the Beilstein or Customer databases currently installed.</td>
</tr>
<tr>
<td>DBTOKENS</td>
<td>Same contents as DBNAMES.</td>
</tr>
<tr>
<td>DBSYNTAX</td>
<td>List of database syntax codes: Currently always &quot;1&quot;.</td>
</tr>
<tr>
<td>DBACCESS</td>
<td>List of database access modes:</td>
</tr>
<tr>
<td>A</td>
<td>Read/Write access.</td>
</tr>
<tr>
<td>R</td>
<td>Read access.</td>
</tr>
<tr>
<td>N</td>
<td>No access.</td>
</tr>
<tr>
<td>NA</td>
<td>Read/Write access, but currently disabled.</td>
</tr>
<tr>
<td>NR</td>
<td>Read access, but currently disabled.</td>
</tr>
<tr>
<td>DBMODE</td>
<td>List of database structure modes: Currently always &quot;ORG&quot;.</td>
</tr>
<tr>
<td>CFDIR</td>
<td>List of data structure table names: It must be base file names without a path.</td>
</tr>
<tr>
<td>CONTEXTS</td>
<td>List of entries (letter combinations) designating the contexts available for display and property search in a particular database:</td>
</tr>
<tr>
<td>--------------</td>
<td>--------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Substances</td>
<td></td>
</tr>
<tr>
<td>Reactions</td>
<td></td>
</tr>
<tr>
<td>Citations</td>
<td></td>
</tr>
<tr>
<td>SEARCHES</td>
<td>Likewise formatted list with the contexts available for structural substance or reaction search or for property citation search.</td>
</tr>
</tbody>
</table>
3.3.2.1.7 Command DBSELECT

DBSELECT <database_name>[:<context_letter>]

The command establishes the default database and optionally also the default context required in a number of commands.

For the new database, a /M response line is issued with the following information:

MINSEQ  minimum entry sequence number, always 1
MAXSEQ  maximum entry sequence number, equals the number of database entries.
MINBRN  minimum ID number (RegNo) of the database or 0.
MAXBRN  maximum ID number (RegNo) of the database
UPDATE  currently not used.

Unlike prior versions, the server does not delete temporary hitsets when selecting a different database.

Example:
@XFIRE>
dbselect BS040300ae
/M MINSEQ=1,MAXSEQ=8932531,MINBRN=0,MAXBRN=9549830,UPDATES=0
@XFIRE>

3.3.2.1.8 Command DELCOMP

DELCOMP <Customer RegNo>

An entry in the current customer database is removed. The user must have write permission to the RegNo given in the command.

Example:
@XFIRE>
DELCOMP 1001
@XFIRE>

3.3.2.1.9 Command DELETE

DELETE <hitset_name>

The current command deletes a temporary or permanent hitset.

@XFIRE>
DELETE q01
@XFIRE>
3.3.2.1.10 **Command DIR**

DIR [ALL]
The DIR command either lists all hitsets from the current database (ALL clause absent) or any hitsets available (ALL present). Using ALL also adds the database name and context.

The table returned has the following columns:

- Hitset name. Current database information is included under a pseudo hitset name DATABASE.
- Number of hits.
- Type of query: F = factual (property), S = structural, U = undetermined.
- Database name and context. Only when ALL is specified.

**Example:**

```plaintext
@XFIRE>
dir all
// HITSET Q01          1029 F BS040300AE:C
// HITSET Q02          1141 F BS040300AE:S
// HITSET Q03           151 F BS040300AE:R
// HITSET DATABASE  6546266 U
@XFIRE>
dir
// HITSET Q01          1029 F
// HITSET Q02          1141 F
// HITSET Q03           151 F
// HITSET DATABASE  6546266 U
@XFIRE>
```

3.3.2.1.11 **Command DOWNLOAD**

DOWNLOAD <hitset_name> <lower_limit> <upper_limit>
The current command retrieves the ID numbers (i.e. BRNs, Customer RNs, reaction IDs, or citation IDs) from a range of hits in a hitset. Hit numbers start at 1. The range specified may extend beyond the number of hits in the hitset.

Output lines begin with a header line providing the first hit number (POS) and the range requested (SIZE). Subsequent lines contain a comma-separated list of ID numbers.

**Example:**

```plaintext
@XFIRE>
DOWNLOAD q01 1 10
//POS=1,SIZE=10
//1001,1002,1003,1004,1005,1006,1007,
//1008,1009,1010
@XFIRE>
```
**Command EXIT**

The EXIT command terminates a session. All temporary hitsets generated during the session are removed. When operating the server from a terminal or in batch mode, end-of-file or Ctrl-D (AIX) is equivalent.

### 3.3.2.1.12 Command EXPAND

**EXPAND** `<field_name> [=<value>] [LINES=<integer>]`  

**EXPAND SEEK=<integer> [LINES=<integer>]**

The EXPAND command renders a section of the index on a searchable database field.

The first form requires a field name from the data structure table (DST) of the current database. It must be a 3-character field name type. The starting value of the index listing may be optionally specified. If this string is to contain blanks or double quotation marks, it has to be enclosed in double quotations marks after doubling all contained double quotation marks. The LINES clause limits the number of output lines (default: 20).

The second form positions to a specific index entry identified by its sequence number. The index to access must have been identified by a prior EXPAND command with a field name.

The command output consists of a header line with the current index position (POS: for the first data line) and the total index size (SIZE). Following is a table of frequencies and field value (after V=).

**Example:**

```bash
@XFIRE>
exp ci2=m lines=5
//POS=288789,SIZE=550068
//1 V=m burnett,g.
//1 V=m'-cullagh
//1 V=m'bairaroua, oubadjim
//2 V=m'bida, abderrahim
//1 V=m'bossa, c.
/OK
@XFIRE>
exp seek=2000 lines=5
//POS=2000,SIZE=550068
//1 V=abraham, raymond
//68 V=abraham, raymond j.
//1 V=abraham, robert
//1 V=abraham, sir edward p.
//5 V=abraham, tonson
/OK
@XFIRE>
```
3.3.2.1.13 Command FINDGAP
The FINDGAP command returns the lowest RegNo in the current Customer database that is unused and may be written to by the current user. If no such RegNo exists, zero is returned.

Example:
@XFIRE>
FINDGAP
// 1002
@XFIRE>

3.3.2.1.14 Command GETCFDIR
GETCFDIR <datastructure_table_name> [<first_line> <last_line>]
The GETCFDIR command returns a range of lines from a datastructure table file (DST) stored at the server. The file name must be specified without a path. If the line number range is outside the lines present in the DST file, nothing is returned.

If line numbers are zero or omitted, the output renders the version number of the DST file.

Example:
@XFIRE>
getcfdir xfaeco7.dst
//VERSION=4.06;
@XFIRE>

3.3.2.1.15 Command REPCOMP
REPCOMP <Customer RegNo>
The REPCOMP command works identically to the ADDCOMP command with one exception: An existing entry under the RegNo specified is replaced.

Example: see ADDCOMP
3.3.2.1.16 **Command REPORT**

The REPORT command works differently for Beilstein / Gmelin and Customer databases:

For a Beilstein database, it renders the same information as is issued by the DBSELECT command (see 3.7).

For a Customer database, a data line is added providing the ranges of entry sequence numbers and ID numbers (Customer RegNos) where the current user (name also provided) has write permission.

**Example 1: Beilstein database**

```
@XFIRE>
report
/M MINSEQ=1,MAXSEQ=8861806,MINBRN=0,MAXBRN=9476792,UPDATES=0
@XFIRE>
```

**Example 2: Customer database**

```
@XFIRE>
report
/M MINSEQ=1,MAXSEQ=120,MINBRN=1060,MAXBRN=10100,UPDATES=0
// MINSEQ=100,MAXSEQ=120,MINBRN=10001,MAXBRN=10100,USER=xfusr
@XFIRE>
```

3.3.2.1.17 **Command RNSEQ**

```
RNSEQ <ID_number>
```

The RNSEQ command operates in the substance or reaction context of a Beilstein or Customer database (using the default settings by a prior DBSELECT): It returns the sequence number at which the specified ID number is present in the sorted set of database ID numbers, or 0 if it is not in use. ID numbers with no structure stored for the substance or reaction are not counted.

**Example:**

```
@XFIRE>
RNSEQ 1001
// 1
@XFIRE>
```
### Command SEARCH

**COMMAND SYNTAX: BEILSTEIN OR GMELIN DATABASE**

SEARCH [FROM <database>] [INTO [hitset]][:<context>]]
[ORIG <text>] <query>
<query> ::= <boolean_query> | <BSD_query>

The SEARCH command provides an interface to all of the server search facilities. It consists of the following clauses:

<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FROM</strong></td>
<td>The database to search in may be specified here. If omitted, the default database from a prior DBSELECT command is searched.</td>
</tr>
<tr>
<td><strong>INTO</strong></td>
<td>The INTO clause is required to specify the context (single letter for Substances, Reactions, or Citations) of the hitset resulting from the query. Optionally, the future hitset may be named using a valid permanent hitset name: 1 to 8 letters or digits, leading letter not only digits after a leading q. The INTO clause may be omitted if the current database has only one context or if the default context established by DBSELECT is desired.</td>
</tr>
<tr>
<td><strong>ORIG</strong></td>
<td>The ORIG clause specifies the “display query” returned by a later UNLOAD command when a Boolean query is used. If the string contains blanks or double quotes, the entire string must be put into double quotes, and the quotes must be doubled.</td>
</tr>
<tr>
<td><strong>&lt;query&gt;</strong></td>
<td>The query may be either a Boolean expression combining restrictions with 3-character field names or a BSD string (Beilstein Structural Data), which in turn may contain a structural query (on substances or reactions), a Boolean query, or both.</td>
</tr>
</tbody>
</table>
Boolean queries may appear in two formats:

The search format, which is actually used during the search.

The display format, which is in 1:1 correspondence to the search format.

Both formats have the same syntax using different operators, delimiters, and quotation rules:

\[
<\text{boolean}\_\text{query}> ::= <\text{clause}> \{ <\text{logical}\_\text{operator}> <\text{clause}> \}
\]

\[
<\text{clause}> ::= <\text{opening}\_\text{parens}> <\text{restriction}> <\text{closing}\_\text{parens}>
\]

\[
<\text{restriction}> ::= <\text{field}\_\text{name}> [ <\text{relational}\_\text{operator}> <\text{value}> [ <\text{from}\_\text{to}\_\text{operator}> <\text{upper}\_\text{limit}> ] ]
\]

\[
<\text{restriction}> ::= .<\text{hitset}\_\text{name}>
\]

A restriction may specify an isolated field name, a field name plus value or range, or a hitset name. All 3 types uniquely belong to a context.

Field names belong to 1 of 3 basic categories:

data field name

property name

search term name

Data fields and properties have been addressed in chapter 2. Search terms are related to certain sets of properties. Their presence for a data item indicates that at least one member property is present.

A value or range selects all data items containing a property with the specified data field being present with a value matching the criterion. Consequently, only data fields may be searched by value.

An isolated field name is allowed only in the display format. It selects those data items in the specific context which contain the named property at least once. Omission of the field value is only allowed for properties and search terms, not for data fields. Converted to the search format, an isolated field name is translated to a representation described below.

Using a hitset implies the target context of an earlier query. The following components are interpreted depending on the query format:
<table>
<thead>
<tr>
<th>Element</th>
<th>Search Format</th>
<th>Display Format</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>&lt;field_name&gt;</code></td>
<td>3-character name (see chapter 5)</td>
<td>short name (see chapter 5)</td>
</tr>
<tr>
<td><code>&lt;logical_operator&gt;</code></td>
<td>und, oder, ohne, link</td>
<td>and, or, not, proximity</td>
</tr>
<tr>
<td><code>&lt;relational_operator&gt;</code></td>
<td>:</td>
<td>&gt;=, &lt;=, &gt;, &lt;</td>
</tr>
<tr>
<td></td>
<td>=&gt;, &lt;:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(not available)</td>
<td></td>
</tr>
<tr>
<td><code>&lt;from_to_operator&gt;</code></td>
<td>=</td>
<td></td>
</tr>
</tbody>
</table>

The logical and relational operators in the display format column may be interpreted in the usual notation. The *proximity* operator may only join elementary restrictions on fields belonging to the same property. It imposes the additional restriction that both requested field values must reside in the same occurrence of the common property. Improper use of this operator will yield zero hits.

Quotation is required as soon as a `<value>` or `<upper_limit>` is to contain characters from an excluded set:

<table>
<thead>
<tr>
<th>Search Format</th>
<th>Display Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>The excluded set is blank, backslash, round parentheses, colon, greater-than, less-than, and equal sign. A character from this set has to be preceded by a backslash.</td>
<td>The excluded set is blank, double quote, and round parentheses. The value containing one of these characters has to be enclosed in double quotes after doubling contained double quotes. In addition, quotation is required when a <code>&lt;from_to_operator&gt;</code> separates two non-numeric values.</td>
</tr>
</tbody>
</table>

Both formats include the wildcard characters ‘?’ (any single character) and ‘*’ (any number of any characters) for text pattern matching.
A restriction without a field value in the display query format has to be translated to the search format:

<table>
<thead>
<tr>
<th>Search Format</th>
<th>Display Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;property_name(display)&gt;</td>
<td>&lt;FA_field&gt;:&lt;property_name(search)&gt;*</td>
</tr>
<tr>
<td></td>
<td>The property name (search format) is searched at the start of a special “field availability” field.</td>
</tr>
<tr>
<td>&lt;term_name(display)&gt;</td>
<td>&lt;Term_field&gt;:&lt;term_name(search)&gt;</td>
</tr>
<tr>
<td></td>
<td>The search term name (search format) is searched as full contents of a second special field.</td>
</tr>
</tbody>
</table>

**COMMAND SYNTAX: CUSTOMER DATABASE**

Customer databases are treated identically when using a query in BSD format. However, the Boolean query component has the following restrictions:

The Boolean query component may consist of a single hitset. It must be combined with a structural query component.

The Boolean query may be a logical combination of two hitsets by and, or, or not. An additional structural component is optional.

Boolean queries outside BSD do not support the FROM and INTO clause. Such queries must consist of two hitsets linked by and, or, or not (also in the search format!).
**COMMAND EXECUTION**

The various components in a search command are executed in the following sequence:

If a Boolean query is present, it is executed first: The query may be viewed as a tree with elementary restrictions as leaves. Each restriction yields an intermediate result set. Result sets are intersected or united to a final result.

The Boolean query result is possibly switched to the context of the structural query component if present. Otherwise, it is switched to the destination context from the INTO clause. The resulting intermediate or final hitset is kept as a temporary hitset.

If both query components are present, the Boolean query result is loaded as a filter on the hits of the structural query subsequently run. Otherwise, the structural query runs without further restrictions. In both cases, the structural query result is possibly switched to the requested destination context.

Both the intermediate and final hitset are reported in /M message lines rendering the following parameters:

<table>
<thead>
<tr>
<th>HITS</th>
<th>Number of hits</th>
</tr>
</thead>
<tbody>
<tr>
<td>NAME</td>
<td>Hitset name</td>
</tr>
<tr>
<td>DB</td>
<td>Name of the database</td>
</tr>
<tr>
<td>CTX</td>
<td>Context of the hits</td>
</tr>
</tbody>
</table>

**Example 1:** Boolean query outside BSD

```
@XFIRE>
search into q01:s ORIG "mp=400-500" ff1:400=500
/M HITS=1674,NAME=Q01,DB=BS040300AE,CTX=S.
/OK
/U CPU 0.41 sec
/U ELA 1.00 sec
@XFIRE>
```

**Example 2:** Boolean query within BSD

```
@XFIRE>
search into :s 
<BSD@<FCT@<FCTORIG="mp=400-500"@FCTRB="ff1:400=500"@CTX=S@TYPE=FCT>@FCT>@ 
>BSD@
pass: search into q01:s ORIG "mp=400-500" ff1:400=500
/M HITS=1674,NAME=Q01,DB=BS040300AE,CTX=S.
/OK
/U CPU 0.44 sec
/U ELA 1.00 sec
@XFIRE>
```
Example 3: BSD reaction query

@XFIRE>
search into :r \n<BSD@<RXN@DIRECTION=FORWARD@<STR@ROLE=PRODUCT@ROSDA=L=1 (X1702,Y1777),2 (X1\n700,Y3250),3 (X2999,Y4000),4 (X4298,Y3250),5 (X4325,Y1777),6 (X2999,Y1000),7\n*(X5624,Y4027),8 (X6923,Y3277),9 (X6923,Y1777),10 (X5624,Y1027),1=6-5=10-9=\n8-7=4-5,1-2=3-4.@AC=7.0@<STR@>RXN@>BSD@

Calling Screening
*** At the moment, allow at most 2 screening sets! ***
1 selected start-atoms:
  Atom: 1  Rank0: 0.00235171  Rank: 0.000415374

Current startatom = 1

Level 0 ... S: 1=> 396 (5319) C: 64045788 Cs: 64045788 (186545808)
  H: 0

  E(all): 0.000 < 0.600  E(bund): 0.000 < 0.060
  w(s)= 2127.6 < w(a)=122502224.0  W= 2127.6  Hist: 1.0 < 100.0

Level 1 ... S: 396=> 505 (92920) C: 11732275 Cs: 11732275 (67317488)
  H: 0

  E(all): 0.003 < 0.600  E(bund): 0.003 < 0.060
  w(s)=36324.2 < w(a)=55592440.0  W=38451.8  Hist: 1.0 < 10.0

Level 2 ... S: 505=> 1167 (1410) C: 12201761 Cs: 12201761 (12290446)
  H: 0

  E(all): 0.003 < 0.600  E(bund): 0.000 < 0.060
  w(s)=1060.8 < w(a)=88685.0  W=39512.6  Hist: 1.0 < 5.0

Level 3 ... S: 1167=> 1293 (3334) C: 7587477 Cs: 7587477 (13003918)
  H: 0

  E(all): 0.005 < 0.600  E(bund): 0.000 < 0.060
  w(s)=1800.4 < w(a)=5416441.0  W=41313.0  Hist: 1.0 < 2.0

Level 4 ... S: 1293=> 1009 (4964) C: 3335150 Cs: 3335150 (8118449)
  H: 0

  E(all): 0.013 < 0.600  E(bund): 0.001 < 0.060
  w(s)=2502.8 < w(a)=4783299.0  W=43815.8  Hist: 1.0 < 2.0

Level 5 ... S: 1009=> 450 (8734) C: 385470 Cs: 385470 (3328369)
  H: 0

  E(all): 0.124 < 0.600  E(bund): 0.010 < 0.060
  w(s)=3897.2 < w(a)=2942899.0  W=47713.0  Hist: 1.0 < 2.0

Level 6 ... S: 450=> 425 (1126) C: 27905 Cs: 27722 (281927)
  H: 0

  E(all): 1.732 > 0.600  E(bund): 0.023 < 0.060
  w(s)=630.4 < w(a)=254022.0  W=48343.4  Hist: 1.0 < 2.0

Level 7 ... S: 425=> 461 (626) C: 18570 Cs: 18285 (27724)
  H: 0

  E(all): 2.622 > 0.600  E(bund): 0.019 < 0.060
  w(s)=347.2 < w(a)=9337.0  W=48690.6  Hist: 1.0 < 2.0

Level 8 ... S: 461=> 633 (1290) C: 5103 Cs: 0 (18185)
  H: 0
E(all): 9.657 > 0.600  E(bund): 0.117 > 0.060
w(s)=  597.2 < w(a)=13367.0  W= 49287.8  Hist:  1.0 <
2.0
* EFC Cand(screening):  0 <  967
* All query atoms mapped
+ No more start-atoms available
CPU 16.01 sec
ELA 17.00 sec
1 screen sets generated:
  1:  633 screens, SA = 1,  5103 cand.,     0 hits, ...
Calling final ABAS
candidate 5000
internal Abas time = 0.73 (sec)
5063 candidates processed
5063 candidates, 1793 hits
/HITS=1793,NAME=Q01,DB=BS040300AE,CTX=R.
/U CPU 26.74 sec
/U ELA 27.00 sec
@XFIRE>

Example 4: BSD combined query: Boolean query plus substructure query.

@XFIRE>
search into :s \
<BSD<STR<ROSDAL=(1N(X1700,Y4345),2*(X950,Y3049),3(X2450,Y3049),1-3-2-1/
.2>STR<FTCTORIG="au=karabin**"FCTRBF="ci2:karabin**"CTX=C@TYPE=FCT>F\nCT><BSD>
pass: search into q01:S ORIG "au=karabin**" ci2:karabin* 
/M HITS=239,NAME=Q01,DB=BS040300AE,CTX=S.
/OK
subset /xfire/usr/cxusr/3063.168430086/q01.hit loaded
Calling Screening
*** At the moment, allow at most 2 screening sets! ***
1 selected start-atoms:
  Atom:  1  Rank0: 2.03504E-06  Rank: 0.000232159
Current startatom = 1
Level 0 ... S:  1=>  15 ( 3808) C: 2807834 Cs: 2807834 (145853952)
H:  0
  E(all): 0.000 < 0.600  E(bund): 0.000 < 0.060
  w(s)=  157.2 < w(a)=143046144.0  W= 157.2  Hist:  1.0 <
100.0
Level 1 ... S:  15=>  52 ( 5051) C:  393 Cs:  0 ( 3000967) H: 393
  E(all): 272.000 > 0.600  E(bund): 114.800 > 0.060
  w(s)=  114.8 < w(a)=3000574.0  W= 272.0  Hist:  1.0 <
10.0
* Cand. processed by Abas =  0 <  2066
* EFC Cand(screening):  0 <  897
* All query atoms mapped
+ No more start-atoms available
CPU 0.28 sec
ELA 1.00 sec
1 screen sets generated:
  1:  52 screens, SA = 1,  393 cand.,  393 hits, ...
Calling final ABAS
0 candidates processed
392 candidates, 1 hits
/M HITS=1,NAME=Q02,DB=BS040300AE,CTX=S.
/U CPU 3.89 sec
/U ELA 4.00 sec
@XFIRE>
3.3.2.1.19  Command SEND or TYPE

COMMAND DESCRIPTION
SEND <data_source> [FROM [<database>][::<context>]] [<view>] [<options>]
<data_source> ::=  <hitset_name>
|  <ID_number>
|  #<sequence_number>
/view> ::=  <view_item> {<view_item>}
/view_item> ::=  #<property_name>[(<low>[:<high>])]
/options> ::=  <option_item> {<option_item>}
<option_item> ::=   RANGE <integer>
|   AUTOSELECT
|   POSTALL
|   HITINFO
|   BYTES=<integer>

The SEND command retrieves a set of properties from a particular data item, i.e. a single substance, reaction, or citation. It has the following components:

<p>| &lt;data_source&gt; | The data item is either a particular hit in a hitset (specified by RANGE) or a database entry selected by its ID number or sequence number. |
| FROM | This clause is used to specify a database different from the current default. It is required if a hitset to address does not belong to the current database. The context specification is ignored when the data source is a hitset. In the other cases, the specification will select a context different from the current default context (from a prior DBSELECT). |
| &lt;view_item&gt; | Any single view item names a property of the current data item by its 3-character name. The third character may be omitted. What follows is an occurrence number or range to be retrieved for the current property. Omission yields all occurrences of the property. The structure of a substance or reaction is named “STR”. An empty view renders all properties of the current data item. |</p>
<table>
<thead>
<tr>
<th>Clause</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>RANGE</strong></td>
<td>The range clause identifies a particular hit in a hitset as the data item for retrieval.</td>
</tr>
</tbody>
</table>
| **AUTOSELECT** | The current clause causes inclusion of only those properties selected by the view which contain a field value matching one of the query restrictions. If the property has one or more citations attached, this field value may instead be located in one of the citations.

The matching field values are enclosed in a pair of highlight symbols - see below. If the query giving rise to the hitset includes a substance or reaction (sub)structure, full structure atoms and bonds mapped onto query nodes are also highlighted. |
| **POSTALL** | This clause works only when accompanied by AUTOSELECT: The omission of properties does not occur, only highlighting is done.                     |
| **HITINFO** | The HITINFO clause renders a field availability list (see next section) including only those properties that carry a highlight, i.e. match the AUTOSELECT condition. |
| **BYTES=** | The size specified limits command output: Before reaching the size, the server prompts back using a string. The user may request continuation sending the next data block by entering n<return> or <return> or cancellation by b<return>. |

**OUTPUT DESCRIPTION**

Output to a send command is a data stream wrapped into the line delimiters “///” (begin) and “@+” (end). This data stream is subdivided by the following strings (which may not be contained in data values):

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>@:</td>
<td>Field name initiator. Following is the 3-character name of a data field (see chapter 5) and the field content. The field value extends up to before the next @: or @; sequence.</td>
</tr>
<tr>
<td>@;</td>
<td>Property delimiter. The preceding fields back to a prior @; or start of data belong to a common property.</td>
</tr>
<tr>
<td>@.</td>
<td>Data unit delimiter. The preceding properties back to a prior @. or start of data belongs to a common substance, reaction, or citation.</td>
</tr>
<tr>
<td>@*</td>
<td>Highlighting symbol. Used to enclose a field value matching a query restriction.</td>
</tr>
</tbody>
</table>
Within a substance, reaction, or citation, the following properties have a special meaning:

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID property</td>
<td>The ID property occurs exactly once per substance, reaction, or citation. It contains a field with the ID number (primary key) of the current data item.</td>
</tr>
<tr>
<td>Structure</td>
<td>A structure with name STR is present for substances and reactions. It is not listed in the field availability (see next).</td>
</tr>
<tr>
<td>Field availability</td>
<td>The field availability property has a single data field named (3-character names) FA_, RA_, or ZA_ for substances, reactions, and citations, resp.</td>
</tr>
<tr>
<td></td>
<td>It is a comma-separated list of entries made up of the 3-character names and occurrences of all properties belonging to the current data item. The structure, field, and search term availability are excluded.</td>
</tr>
<tr>
<td></td>
<td>Example: @:FA_CT_8,GZ_3@;</td>
</tr>
<tr>
<td>Search term availability</td>
<td>The search terms for a substance make up the contents of a special field: it is a comma-separated list of their 3-character names.</td>
</tr>
</tbody>
</table>

The HITINFO clause described above yields the names and occurrence numbers of those properties of a data item, which contain fields matching a search restriction. The ID property is always included. It’s format may be seen from the following example:

```
@:HITID_1;FF_2,3,4;@;@:HIT { <name> <index> {, <index> } ; } @;
```

If a property refers to citations, all those citations are issued after the property data itself. Any single citation ends in the property delimiter “@;“.

When included in substance or citation context, reactions appear as a single property merged from the original ID property and a particular reaction details property with no intervening delimiter. In substance context, the citation reference follows the reaction details.
Example:

A combined query is done joining the property restriction “mp=400-500” with a substructure. It yields an intermediate hitset q01 from the property query part. The hitset q01 is then searched giving rise to the final hitset q02.

All properties of the first hit are displayed.

@example>
search into :s \
<BSD@<STR@<ROSDAL=()1*(X1447,Y1004),2*(X1447,Y1840),3(X2171,Y586),4N(X217\1,Y2257),5N(X2895,Y1004),6O(X2174),7(X2895,Y1840),8O(X3500,Y2243),1-3=6,\1-2-4-7=8,3-5-7.0>STR0<FACTORIG="mp=400-500">FACTRB="ff1:400=500">CTX=\S@TYPE=FACT0>BSD@ 
/M HITS=1674,NAME=Q01,DB=BS040300AE,CTX=S. 
/OK subset /xfire/usr/cxusr/16271.168430086/q01.hit loaded Calling Screening 
*** At the moment, allow at most 2 screening sets! *** 1 selected start-atoms: 
Atom: 8  Rank0: 5.49788e-06  Rank: 8.52006e-06 Current startatom = 8 
....
CPU 1.90 sec

ELA 2.00 sec 1 screen sets generated: 
1: 443 screens, SA = 8, 6377 cand., 5741 hits, ...
Calling final ABAS candidate 
3 candidates processed 
6277 candidates, 4 hits
/M HITS=4,NAME=Q02,DB=BS040300AE,CTX=S. 
/U CPU 3.11 sec
/U ELA 4.00 sec
@example>
send q02 range 1 autoselect postall 
//@:ID18145@:IDX21038-67-5@:ID321038-67-5@:ID51#H!-pyrido<3,4-#d!>pyrimidin@+ 
//ne-2,4-dione@:ID91#H!-pyrido<3,4-#d!>pyrimidine-2,4-dione@:IDA0-26-00- 
00@+ 
//236@:IDA4-26-00-00578@:IDA5- 
26@:IDDC.....7H.....5N.....3O.....2@:IDJI63.0+ 
//140:ID430139@:IDFC.....7@:IDFH.....5@:IDFN.....30:IDF0.....20:IDI1@:IDG 
10@+ 
//70:IDH4@:IDVheterocyclic@:IDLand 
tautomers@:IDM88.06.270@:IDN92.01.310;@:0+ 
//FA_CT_6,EW_1,FF_6,FU_1,RE_1,SV_1,BL_1;@:CT2Preparation@:CT5cinchomeron 
i@+ 
//c acid diamide@:CT68145@:CT71#H!-pyrido<3,4-#d!>pyrimidine-2,4- 
dione@:CT@+
//Ealkaline hypobromite @CT0807201@:CT0807200@;@:R1_807201@:CI1Journal@:CI0+
//Blumenfeld@:CI7MOCMB7@:CI8Monatsh.Chem.@:CIG160@:CI11895@:CIJ709@;@:R1_80+
//07200@:CI1Journal@:CI2Gabriel;
Colman@:CI7CHBEAM@:CI8Chem.Ber.@:CIG350@:C0+
//II1902@:CIJ2844,2847@;@:CT2Preparation@:CT53-amino-pyridine-carboxylic
a@+
//cid-(4)@:CT4635724@:CT5urea@:CT681450@:CT71#H!-pyrido<3,4-
d!pyrimidine-8+
//2,4-dione@:CTJ1700@:CT0807202@;@:R1_807202@:CI1Journal@:CI2Gabriel;
Colma@+
//n@:CI7CHBEAM@:CI8Chem.Ber.@:CIG350@:CI11902@:CIJ28360@;@:CT2Preparation@:
C0+
//T681450@:CT71#H!-pyrido<3,4-&d>pyrimidine-2,4-
dione@:CT027613470@:CT027610+
//4018@:CT027614020@:CT05196547@;@:R1_2761401@:CI1Patent@:CI3Sherwin-
Williams@+
//s Corp.@:CI4US 3887550@:CI519750@:CI9Chem.Abstr.@:CICEN@:CIF83@:CIH147504@
//@;@:R1_2761401@:CI1Patent@:CI3Sherwin-Williams@:CI4US
3947442@:CI519760@:C0+
//CI9Chem.Abstr.@:CICEN@:CIH5683@;@:R1_2761402@:CI1Patent@:CI3Sher
w@+
//in-Williams@:CI4US 3947416@:CI519760@:CI9Chem.Abstr.@:CICEN@:CIG850@:CIH33@
/@;@:R1_5196547@:CI1Journal@:CI2Beckwith;
Hickman@:CI7JSOOAX@:CI8J.Chem.Soc.0@:CIG756@;@:AX_@+
//m.Soc.C@:CIG11960@:CIJ27560@;@:CT2Chemical behaviour@:CT481450@:CT51#H!-
pyr@+
//ido<3,4-&d>pyrimidine-2,4-dione@:CT5hydrochloric acid@:CT73-amino-
pyrid@+
//ine-carboxylic acid-(4)@:CTJ180 -
190@:CT08072010@:CT08072008@;@:R1_8072010+
//m.Ber.@:CIG350@:CI11902@:CIJ2844,2847@;@:CT2Chemical
behaviour@:CT481450@:C0+
//CT51#H!-pyrido<3,4-&d>pyrimidine-2,4-
dione@:CT05196547@;@:R1_51965470@:C0+
//IIJournal@:CI2Beckwith;
Hickman@:CI7JSOOAX@:CI8J.Chem.Soc.C0@:CIG11968@:CI0+
//J27560@;@:CT2Chemical behaviour@:CT481450@:CT51#H!-pyrido<3,4-
#d!pyrimidi0+
//ne-2,4-dione@:CT01977440@;@:R1_1977440@:CI1Journal@:CI2Gelling, I.R.;
Wibbe@
//rley,D.G.0@:CIG17JSOOAX@:CI8J.Chem.Soc.C0@:CICEN0@:CIJ931-
9340@;@:AX_@+
//ZA,AM, ZH-, ZE-, ZRE, ZR_ @;@:EW1gelblich@:EW08072000@;@:R1_8072000@:CI1Jour
n0+
//a0@:CI2Gabriel;
Colman@:CI7CHBEAM@:CI8Chem.Ber.@:CIG350@:CI11902@:CIJ28440+
//,28470@;@:FF1365@:FXnach Sublimation bei 210grad/0.01
Torr.0@:FF0818271@;@+
//@;@:R1_8182710@:CI1Journal@:CI2Beckwith;
Hickman@:CI7JSOOAX@:CI8J.Chem.Soc.0+
3.3.2.1.20 Command SEQRN

SEQRN <sequence_number>

The SEQRN command inverts the function of the RNSEQ command: It yields the ID number at the position specified within the sorted sequence of all database ID numbers. Only substances or reactions with a structural representation are counted.

Example:

```
@XFIRE>
SEQRN 1
// 1001
@XFIRE>
```

3.3.2.1.21 Command SET

The SET command is reserved for internal debugging use.

3.3.2.1.22 Command SM

The SM command is supported for backward compatibility only. It prompts for the entry of a Rosdal string query. Multiple lines with no continuation character are expected. The final line should close with an at sign (@).

Example:

```
@XFIRE>
SM
@SM>
1--6-
@SM>
1.@
...
@XFIRE>
```

3.3.2.1.23 Command STORE

STORE <source_hitset> INTO <target_hitset>

This command copies an existing hitset to a new hitset. Hitset names consist of 1 to 8 letters (no case sensitivity) or digits with a leading letter. Hitset names starting with Q and otherwise consisting of digits are reserved for temporary hitsets and illegal as target names.

Example:

```
@XFIRE>
STORE q01 INTO myhitset
@XFIRE>
```
3.3.2.1.24 Command UNLOAD

UNLOAD <hitset_name>

The UNLOAD command retrieves the query which gave rise to a hitset. The query is rendered as a data stream wrapped into data lines.

Example:

@XFILE>
unload q01
//1--6-1.00+
@XFILE>
3.3.3 THE CROSSFIRE DISPATCHER “XFDISP”

CrossFire dispatcher is a communication tool that handles the communication between the CrossFire clients (MDL CrossFire Commander) and the MDL CrossFire Server software. It also handles encryption, if enabled. One dispatcher belongs to every client/server combination.

3.3.3.1 General

XFDISP calls the program XFLOG for authentication and XFLOG will return exit codes. If XFLOG returns “0” then the connection will be established and the MDL CrossFire Server will be loaded. If XFLOG returns a “2” or “3” exit code, then the connection attempt will be rejected. Please refer to section on XFLOG for details on the exit codes.

XFDISP will pass over the user-id and the password to XFLOG together with additional server options (please refer to the chapter on XFLOG on details for these server options). If the password contains characters, which are not alphanumeric, then it will be encrypted using the following method (C-code example):

```c
#include

#define PWDSET "\abcdefhijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789"

static void protect ( char** s )
{
    UINT len ; char* t = NULL ; char* p, *q ;
    if ( !s || !*s || (len = strlen(*s)) == strspn ( *s, PWDSET )
        || len > UINT_MAX/4
        || !(t = new char[2*len+3]) )
        return ;
    else
        strcpy ( t, "__" ) ;
    for ( p = *s, q = t+2 ; *p ; ++p )
        q += sprintf ( q, "%02X", (BYTE) *p ) ;
    delete[] *s, *s = t ;
}
```

/******************** invert the protection ********************/
void unprot ( char* s )
{
    char *p; char t[3] = "XX"; UINT code;
    if ( !s || !*s || memcmp ( s, "__", 2 ) ) return;
    for ( p = s, s += 2 ; *s ; )
    {
        memcpy ( t, s, 2 );
        sscanf ( t, "%X", &code );
        *p++ = code;
        if ( *++s ) ++s;
    }
    *p = 0;
}

If you want to write and use your own XFLOG program, then you need to be able to interpret the output of XFDISP. Please use the above C-code for writing a parser for the password output of XFDISP.

**Note:** XFDISP is able to work with a modified version of XFLOG which is able to return two different user names instead of the original login name. XFDISP will then use the first of this user names instead of the login user name for accounting.
3.3.3.2 Commands

The following commands are used for the communication between the CrossFire daemon and CrossFire dispatchers/servers through the license port (default 8003).

3.3.3.2.1 Command INTHelp

**INTHelp**

Server help.

Will display a description of server commands

3.3.3.2.2 Command GETParm

**GETParm**

<pgm> <db> <root>[!<option>]

Support for old and new clients:

- The `<option>` contains the name of the group and the command will respond back the name of the server program (<pgm>) and the CrossFire root directory (<root>), which belongs to this group.
### 3.3.3.2.3 Command Ports

**PORTS**

Send ports: client, accounting, licensing, control.

Will return the port numbers of the CrossFire system.

### 3.3.3.2.4 Command LOGIN / LOGOUT

**LOGIN**

\(<pid> \ <user> \ <option>, \ option \ is: \ GROUP=...;STATION=...;CLIENT=...;IPADDR=...;\)

Registering a user at the CrossFire daemon by the MDL CrossFire Server:

<table>
<thead>
<tr>
<th>pid</th>
<th>Process ID number of the server</th>
</tr>
</thead>
<tbody>
<tr>
<td>user</td>
<td>User name</td>
</tr>
<tr>
<td>GROUP</td>
<td>Group name</td>
</tr>
<tr>
<td>STATION</td>
<td>ID of the workstation or empty</td>
</tr>
<tr>
<td>CLIENT</td>
<td>Name of the workstation or empty</td>
</tr>
<tr>
<td>IPADDR</td>
<td>IP address of a workstation or empty</td>
</tr>
</tbody>
</table>

**LOGOUT**

\(<pid>\)

Cancellation of a user, releases a license.

### 3.3.3.2.5 Command SELECT

**SELECT**

\(<pid> \ [<database>]\)

Selection of an available database out of the license group of the user.
3.3.3.2.6 Command TRYUSE

TRYUSE (<pid>|<group>) <software license name>

Response to the request, whether a process or a group has licensed a specific software.

3.3.3.2.7 Command SHOWPROD

SHOWPROD <pid> : Show available stations for group of pid.

Will return the number of free stations licenses for a single product in the license group of the registered user.

3.3.3.2.8 Command REGSTAT

REGSTAT <pid> <product>

The registered user is using a free station license for a product of his current license group. A station id, valid for this license group, must be entered during the login process.
3.3.4 THE CROSSFIRE AUTHENTICATION TOOL “XFLOG”

The dispatcher XFDISP launches this program together with various parameters (see below) as soon as a client tries to login to the server. It checks the authentication of the user and returns exit codes. Depending on the exit code the dispatcher then decides whether a user is allowed to use the system or not.

A program written by the system administrator can replace the standard XFLOG program. The version delivered by MDL is using the operating system feature for authentication. A customer program may use another method but the program needs to reply exit codes as expected.

Usage:

```
xflog <user> <password> [new_password] [-o<server_options>]
```

The parameters [new_password] and [-o<server_options>] are optional. However, XFDISP will send them in any case (new password only if a user has entered it) and a customized XFLOG program may use them for various purposes.

The following server options will be sent to XFLOG:

- GROUP=<license group name>;
- STATION=<station id>;
- CLIENT=<station name>;
- IPADDR=<TCP/IP address of the client>;
- SEED=<alphanumeric string>;
- MASTER=<TCP/IP address of the master server or empty>;

Example:

```
-oGROUP=test;STATION=PAB23IIRMVKU16IGJ3VTG8GAVLTIVL69V0TPV0H877
HU76H3PCSO74H4PN;CLIENT=test_station;IPADDR=10.10.0.255;SEED=ed5
33c2d1e9b6da0b2ed875a07a18;MASTER=;
```

The possible output messages of XFLOG as expected by XFDISP are the following:

stdout message: TRUE (OK), FALSE, or EXPIRED
exit code: 0 (OK), 2 (ERROR), or 3 (EXPIRED)

A self written version of XFLOG could be able to return two different user names. One of them may be the login name, but this is not necessary.

orig. UserID > CrossfireUserID, Ident_UserID
The two UserIDs should be separated by a | symbol. XFDISP will use the first
returned user name (here called CrossfireUserID) instead of the login user name
(orig. UserID) to start the CrossFire process. This can be used to force a user into a
specific user group on the AIX machine. The second returned user name (here called
Ident_UserID) will be used for accounting. If only one UserID is returned it will be used
for both purposes.

The output of XFLOG would look like the following:

stdout message: user name (OK), FALSE, or EXPIRED
exit code: 0 (OK), 2 (ERROR), or 3 (EXPIRED)

Under AIX it is also possible to use a NON-NIS authentication (“yellow pages”). Only if
this is installed on the system XFLOG needs to know this. It gets to know it by setting
a system variable BEFORE xfired is started. Enter the following command before you
start xfire:

export XFLOG_YP=Y

3.3.5 THE CROSSFIRE ACCOUNTING TOOL “XL_STAT”

This tool can be used for the analysis of accounting files: it summarizes all entries of a
single user.

xl_stat <accounting log file name>

The output will be written to the screen. You may capture this output using a pipe
command to a file.
3.3.6 THE CROSSFIRE MAINTENANCE TOOL “XFMAINT”

XFMAINT is the basic maintenance tool of the CrossFire system. It is used for installing the databases, for verifying installations and for creating customer databases. XFMAINT can be launched with a parameter, which contains the CrossFire root directory, e.g.:

```
xfmaint /xfire
```

If you do not specify the CrossFire root directory, you will be asked to confirm the default directory:

```
[xfireadm@dbd-aix-ff1:/xfire/sys] xfmaint
XFMAINT: Database maintenance utility
MDL CrossFire Server Software, Version 7.0 (Build 23)
Copyright (c) MDL Information Systems GmbH 1996,2004
Operating system: AIX 4 3

Database maintenance utility session on Tue Feb 24 12:27:34 2004

output is saved in verify.log and verify.err
enter root path (default /xfire):
```

After XFMAINT has started it will present the following main menu screen:

```
[xfireadm@dbd-aix-ff1:/xfire/sys] xfmaint
XFMAINT: Database maintenance utility
MDL CrossFire Server Software, Version 7.0 (Build 23)
Copyright (c) MDL Information Systems GmbH 1996,2004
Operating system: AIX 4 3

Database maintenance utility session on Tue Feb 24 12:27:34 2004

output is saved in verify.log and verify.err
enter root path (default /xfire):
```

```
1    Add or Remove Filesystems
2    Install, Backup, or Remove Database
3    Customer Databases...
4    En/Disable Database
5    Install Incremental Update
6    Build New Database Image
7    Verify Installation
8    Check File Readability
9    Determine Checksums of Installed DBs
10   Give Help
0    Exit

select:
```
From this main menu you may call different services just by typing the number of the service you would like to run.

### 3.3.6.1 Menu Option 1: Add or Remove Filesystems

Using this option, you define the file systems used for the storage of CrossFire databases. File systems intended for CrossFire databases must be created by an authorized user prior to using this option. What you see first is a list of the file systems already defined to XFIRE. You may delete filesystems from that list by typing "r#," with "#" being the sequence number in the leftmost column.

To add a new file system, select "a". A list of all file systems currently mounted is shown. A string “XFIRE” marks file systems already defined to XFIRE in the second column of the table. To the right of that column, there are total and free space, and the mount point of each file system.

To select one or more file systems shown on the current page, enter a (list of) file system number(s) from the leftmost table column, separated by any non-digit character. To proceed to the next page, press return.

**Note - Windows NT:**

If you want to store the database in a specific directory on a drive you have to rename the filessystem with option n#. Enter the directory name together with the drive letter, e.g. “d:\bsdata” and NOT “bsdata”.

Entering a file system name without a drive letter will corrupt the XFIRE.INI file, which then has to be corrected manually.

### 3.3.6.2 Menu Option 2: Install, Backup, or Remove Database

Under this option, you will find facilities to install, backup (from/to tape), or remove a XFIRE database.

1. Database Installation (Option "i")

   Installation starts from a set of tape cartridges. Each cartridge is identified by a label LLL-# where LLL is a string defined at backup time and # is a sequence number 1...N. A database to be installed must have a unique name. This name, plus all files belonging to a database are stored on a file named "filelist," and stored on the first cartridge of the set. After selecting the install option and entering the tape label, you are asked to insert the first cartridge. The program first looks for "filelist" in the /xfire/sys directory which may be still present from an earlier installation. If you are sure that this file list is valid, you may skip retrieving it from tape. Otherwise, it is loaded from tape.
The database identified in the file list (either just copied from tape or present before) must be new. If you intend to continue with a partially installed database, you first have to remove the database from the database list.

The database files identified in the file list are searched by name in all currently available file systems (see option 1). If a file name is found in exactly one system, and if it's size matches the prescribed value stored in the file list, this disk file is accepted as valid and skipped when copying files from tape. If a file has multiple hits or a different size, its name is shown on screen, and the installation stops. You have to delete or rename that file and retry the installation.

All files not yet present on disk have to be retrieved from tape. The program allocates space for all those files using the file systems currently defined under option 1. It will ensure that each file has sufficient space. If the total file system capacity is exceeded, you first will have to add more file systems using option a.

If enough space is available, the program writes a script file named "load.bat" ("load.xfs" in case of Windows NT). You have to quit the program and to execute this script. The script assumes that tape cartridge No. 1 is already inserted. It prompts for insertion of subsequent cartridges. Reading a complete cartridge will take about 2h.

2. Software Installation

Software installation is also initiated using option "i". You are prompted for insertion of the first cartridge of a set. The program will first retrieve a file list and then write a script "load.bat" to copy files from tape to /xfire/bin and /xfire/sys. This will replace all files of the same name.

3. Database Backup

Any database installed may be backed up to one or more tape cartridges. The number of cartridges required and the distribution of files are determined in advance. Software may be included or not. The result is a script "save.bat" to be executed after quitting the program.

4. Database Removal

The remove option "r" deletes a database from the XFIRE configuration file and writes a script "del.bat" to also delete the database files from disk. If you are fixing an installation previously interrupted, it might NOT be necessary to execute that script.
3.3.6.3 Menu Option 3: Customer Databases...

Note1: This option is not required for the use of the CrossFire Beilstein or CrossFire Gmelin databases. Please refer to chapter 3.10.3 for more details on this topic.

Note2: XFIRED has to be stopped before performing this menu option.

3.3.6.3.1 Menu Option 3.1: Create Customer Database

You may install customer databases for structures and reactions. Entries of a customer database are labeled by a number in the range 1...64,000,000. There may be two types of entries:

- Public entries, which are read-only to all XFIRE users. They should be assigned to an entry number range from 1 to an upper limit “n”. The XFIRE administrator by means of option 6 carries out update to such entries.

- Private entries by XFIRE users authorized with write access to a customer database. Each XFIRE user may get assigned a range of database entry numbers for private use. This is done by option 4. Updating, deleting, and browsing of private entries involves the XFIRE client programs.

- Private entries of one user are visible to other users, only after the administrator has applied a collection and loading step, according to options 5 and 6. Under the current options, a new customer database is initialized and provided with a (unique) name. It may be designated for either structures or reactions.

3.3.6.3.2 Menu Option 3.2: Add or Remove User

The current option first shows a list of all customer databases currently defined. After selecting a database, you may list all currently defined update-enabled users of the database, or add or remove a particular user. Note that XFIRE users not permitted for updates may nevertheless browse or search the customer database.

To add a new user, consider the following topics:

- A user may update a range of entries defined by a minimum and maximum entry number. Those ranges must not overlap each other.

- In addition to privates entries assigned to users, a customer database may contain public entries maintained by the XFIRE administrator. The entry number range occupied by public entries must not overlap with any user range. When adding the first user, sufficient space for public entries should be reserved below the lower limit of the first user's entry range.
3.3.6.3.3 Menu Option 3.3: Collect all User Structures
This option is intended to make structures or reactions entered by an XFIRE customer database user, visible to all users, as well as improving search performance.

When a particular customer database is selected under this option, all private user entries entered or modified since the last collect/load operation, are made ready to be copied within the customer database using option 6.

A subsequent load step will move entries currently being searched in display files to a common search file with better search performance.

3.3.6.3.4 Menu Option 3.4: Load Data into Customer File
With option 3.4, you may perform 2 tasks on a customer database:

- Complete a “collect” step initiated using option 3.3.
- Load, replace, or delete public structures (or reactions) with entry numbers outside any user entry range. For the second task, you are prompted for 3 file names. When completing a collect step, simply enter 3 empty lines. The 3 files have the following meaning:
  - SDF file: Each entry to be added or replaced must be present in an SDF file generated by the xfwrap program. Input to “xfwrap” is a text file with one ROSDAL string, or reaction BSD string, per line. Each entry must be provided with a unique ID number according to the respective formats. (ROSDAL: CRN"..." field, BSD: RID=...@ field). Entry numbers must not overlap with any range for private user entries.
  - SEARCH deletion list: Each entry to be replaced or deleted during the intended load step must be represented by a line in a text file. Lines must contain entry numbers in decimal format.
  - DATA deletion list: Each entry to be deleted from the customer database has to be represented by a text file line containing the entry number plus the appended letter ‘D’. Inclusion of entries being replaced is optional.

The XFMAINT program first checks if the currently used file systems provide sufficient space for intermediate and final storage requirements. A script named "load.bat" is written which must be executed after quitting XFMAINT.

3.3.6.4 Menu Option 4: En/Disable Database
An XFIRE database must be disabled prior to the following actions:

- Remove a database (option 2, suboption r).
• Remove a user (option 3.2, suboption r).
• Load data into a customer database (option 3.4).

In addition, a newly installed database starts as disabled. Disabling only works if no XFire user is on the system.

3.3.6.5 Menu Option 5: Install Incremental Update
This option is not yet available in Version 7.0.23.

3.3.6.6 Menu Option 6: Build New Database Image
This option is used to repair a damaged or invalid database image file. Under normal conditions, such files are created automatically using the options "En/Disable Database" and "Install Incremental Update".

However you also need to run this after an update of the CrossFire Server software.

3.3.6.7 Menu Option 7: Verify Installation
Database verification should be done after any major change to the XFire system. Check the file VERIFY.LOG and/or VERIFY.ERR afterwards.

3.3.6.8 Menu Option 8: Check File Readability
This will lead to an extensive database verification, which takes longer as the procedure used under menu option 8, but will give more reliable results. Should be done after any major change to the XFire system.

XFMaint will try to read 1 kb of every MB of a file (small files will be read completely). If an error occurs on file open the process will be terminated. Otherwise it will give an error message (and the position) and the check will continue.

3.3.6.9 Menu Option 9: Determine Checksums of Installed DBs
For all files of a particular database, a MD5 checksum is determined. If a checksum file has been delivered with the database, it is matched automatically detecting corrupt files. If no checksum file was delivered, please call support for it being mailed.
3.3.7 THE CROSSFIRE MANAGER CONTROL PROGRAM “XFMANAG”

3.3.7.1 Introduction

CrossFire Daemon/Manager Control Program XFMANAG has to be used to manage the CrossFire daemon with regard to accounting options, licensing procedures and license group management.

XFMANAG is a command line program, which offers a command prompt once the program has started. At this prompt various commands can be entered in order to maintain the system. These commands are described in this chapter.

XFMANAG will be launched according to the following procedure:

• Change to the CrossFire sys directory
• Start XFMANAG by typing the command xfmanag at the system prompt
• Termination: Bye, exit or quit.

The commands described in the following can be abbreviated as long as the command remains unambiguous.

Note: XFMANAG can also be used in scripts or batch jobs, if xfmanag is called together with a command and its appropriate parameter. XFMANAG will terminate automatically after command execution.

3.3.7.2 List of Commands

The following commands can be entered at the system prompt.

1. Miscellaneous Commands
   • HELP
   • DUMP
   • GET DUMP
   • SET DUMP
   • GROUP
   • USERS
• SET ROOTPATH
• SET USERDIR
• SET PERMDIR
• SET TEMPDIR
• SET TIMEOUT
• SET TRAINING
• SET FILTER
• SET ALERT

• SHOW DATABASES
• SHOW DUMP
• SHOW GROUPS
• SHOW ALERT
• STOP CROSSFIRE
• TEST PERMISSION

2. Licensing Commands

• CLEAR LICENSE
• PURGE LICENSE
• REFRESH LICENSE
• SET LICENSE
• SHOW LICENSE
• TRY LICENSE

3. Accounting Commands

• EXCLUDE COMMAND
• GET LOG
• INCLUDE COMMAND
• NEW LOG
• SHOW COMMANDS
• SHOW LOGNAME
• START ACCOUNTING
• STOP ACCOUNTING
3.3.7.2.1 Miscellaneous Commands

**COMMAND HELP**

HELP <page No.> : Show help page 'No.', def. 1.

Will display help text pages: first page available with „help“ or „help 1“ or „h“, the
following pages will show up by adding the page number, e.g. „h 2“.

*** Help page 1 of 3 ***

HELP <page No.> : Show help page 'No.', def. 1.

SHOW COMMANDS

Show commands being accounted.
If a name ends with an underscore, omit arguments.


STOP ACCOUNTING [/GROUP=group] : Stop accounting XFIRE commands.
Apply to one group or all.

GET LOG (<last>|<all>) : Display the log file contents.
Show the last 20 (default) or (at most) 10000 lines.

NEW LOG

Rename the current log file (new name is shown). Rewrite the current file from its start.

SHOW LOGNAME

Display the current log file name.

INCLUDE COMMAND <command> : Include commands into the log.

EXCLUDE COMMAND <command> : Exclude commands from the log.

DUMP

Dump license files from memory.

USERS [<user>], omit for all.

GROUP [<group>] [/FULL], '*' or omit for all.

STOP CROSSFIRE

Stop the manager and all sessions.

Command parameters in square brackets are optional.
SET DUMP  [/FILE=<filename>] [OFF]:  Dump to file, def. xfmanage.log, or switch off.

GET DUMP                      Show the dump file name.

SHOW DUMP  [/FILE=<filename>] [ALL] Show file, def. current dump file 20 or 10000 lines.

SET LICENSE   [/LOCALFILE=<filename>] [/KEY=<encoded>] [/PRODUCT=...] [/UID=...] [/STATION=...] [/NAME=...] [/GROUP=...][/COUNT=...] : Add or update license.

CLEAR LICENSE  [/PRODUCT=...] [/UID=...] [/STATION=...]
[/GROUP=...][/COUNT=...]: Modify license.

PURGE LICENSE  /GROUP=... : Remove expired licenses.

REFRESH LICENSE /GROUP=... : Make new license state available to users (single or all groups).

SET ROOTPATH  /GROUP=... [/PATH=...]: Change root path for a group. Omit keyword to reset to default.

SET USERDIR   /GROUP=... [/PATH=...]: Change USR directory for a group. Omit keyword to reset to default.

SET TEMPDIR   /GROUP=... [/PATH=...]: Change TMP directory for a group. Omit keyword to reset to default.

SET PERMDIR   [/GROUP=...][/PATH=...]: PERM directory for a group or all. Omit keyword to reset to default.

SET TIMEOUT   [/GROUP=...] /TIME=... : Set timeout for a group or all.

SET FILTER   [/GROUP=...][/FILTER=...]: Set IP filter (2 files) for a group or globally. Omit keyword to remove filter.

TRY LICENSE  [/GROUP=...]: Try loading the current license state for check (single or all groups).

SHOW LICENSE  [/PRODUCT=...][/GROUP=...]: Display license.
SHOW DATABASES        Show all installed databases.
SHOW GROUPS           Show all groups.
SET TRAINING          /GROUP=... /TIME=...:  Set training mode.
TEST PERMISSION       [GROUP=...] [PRODUCT=...] /VALUE=...
                      Test permission for a user or IP address.

*** Help page 3 of 3 ***

SET ALERT             [/TIME=...] [/HITS=...] [/SETS=...] [/RUN=...]
[/EACH=...] [/DATE=...] [/UPDATE=...] [/XUID=...] 
[/MAIL=...] [/FROM=...] [/PORT=...] [/IMSG=...]
[/YPWD=...] [/NUMAL=...] [/ALUSR=...]

                     For alerts: max. time (sec), hits/hitsets per order, 
                     starting time HHMMSS, run interval (days), prior run 
                     date YYYMMDD, update timestamp FF_YYYYMMDD:HHMMSS, 
                     mail server, sender name, SMTP port, initial mail 
                     message, mail UID/PWD, max. total alert count, max. 
                     alerts per user

SHOW ALERT           Show alert parameters.

COMMAND DUMP
DUMP                 license files from memory.

This will display the current content of all license files and filters.

COMMAND GET DUMP
GET DUMP             Show the dump file name.

This will display the name of the capture file.

COMMAND SET DUMP
SET DUMP             [/FILE=<filename>] [OFF]
                     Dump to file, def. xfmanage.log, or switch off
This will start a capture session (no parameter), or start a capture session with writing the output into a specific file (parameter /FILE). The capturing can be stopped with the parameter OFF.
**COMMAND GROUP**

GROUP  

The command GROUP will display short notices to all groups, GROUP <group name> will display short notices to this specific group, GROUP <group name> /FULL will display all available information to a specific group and GROUP */FULL will display all available information to all groups:

<table>
<thead>
<tr>
<th>GROUP</th>
<th>Name of the group</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRODUCT</td>
<td>Name of a licensed product: database or software product</td>
</tr>
<tr>
<td>EXPIRES</td>
<td>Expiration date</td>
</tr>
<tr>
<td>CONCUR.</td>
<td>M (N): Number of the concurrent licenses, which are currently in use (M) and available in the whole.</td>
</tr>
<tr>
<td>NAMED</td>
<td>Number of named user licenses, which are currently in use and available in the whole</td>
</tr>
<tr>
<td>STATION</td>
<td>Number of station licenses, which are currently in use and available in the whole</td>
</tr>
</tbody>
</table>

If the parameter /FULL has been used, the following information will be displayed in addition:

- A list of the names of all defined users and registered stations for a database product will be displayed.

- At the end of a group the available databases for this group will be displayed.
**COMMAND USERS**

**USERS**

[<user>], omit for all.

This will display the following entries for a specific user or all currently logged in users:

<table>
<thead>
<tr>
<th>GROUP</th>
<th>License group</th>
</tr>
</thead>
<tbody>
<tr>
<td>PID</td>
<td>Process ID number</td>
</tr>
<tr>
<td>STATION</td>
<td>Station name or station ID</td>
</tr>
<tr>
<td>IP</td>
<td>IP address of the current connection</td>
</tr>
<tr>
<td>DATABASE</td>
<td>Currently used database or nothing</td>
</tr>
</tbody>
</table>

**COMMAND SET ROOTPATH**

**SET ROOTPATH**

/GROUP=... [/PATH=...]: Change root path for a group.

This command will enter a path keyword into the file XFIRED.CFG. The CrossFire system then expects to find the directories <bin>, <tmp> and <usr> under the specified path. The directory <bin> needs to contain the XFIRE.INI file, but nothing else.

**COMMAND SET USERDIR**

**SET USERDIR**

/GROUP=... [/PATH=...] : Change USR directory for a group.

If the system administrator needs to move the user directory from the default CrossFire system <usr> directory to another location, then the path to this new location should be entered here. XFMANAG will then enter this path in the XFIRED.CFG file.

**COMMAND SET PERMDIR**

**SET PERMDIR**

[/GROUP=...] [/PATH=...]: PERM directory for a group or all. Omit keyword to reset to default.

If the system administrator wants to move the perm directory from the default CrossFire system <usr> directory to another location, then the path to this new location should be entered here. XFMANAG will then enter this path in the XFIRED.CFG file.
COMMAND SET TEMPDIR

SET TEMPDIR /GROUP=... [/PATH=...] : Change TMP directory for a group.

If the system administrator needs to move the temp directory from the default CrossFire system <tmp> directory to another location, then the path to this new location should be entered here. XFMANAG will then enter this path in the XFIRED.CFG file.

With the options Set TempDir and Set PermDir it is possible to separate the disk space for permanent hitsets and for temporary files.

COMMAND SET TIMEOUT

SET TIMEOUT [/GROUP=...] /TIME=... : Set timeout for a group or all.

It is possible to set a specific server timeout for every group of a CrossFire installation or to modify the default timeout of 2 hours. Usually the MDL CrossFire Server will disconnect from a client after 2 hours. If this time needs to be changed then enter the new time out in seconds at this prompt. A "0" will be interpreted as default timeout.

COMMAND SET TRAINING

SET TRAINING /GROUP=... /PRODUCT=... /TIME=...

This command may be used to establish a temporarily increased maximum usage count for a product licensed by a group. Please contact Elsevier MDL if you need such a temporary training license.

COMMAND SET FILTER

SET FILTER /GROUP=... [/FILTER=...] : Set IP filter (2 Files) for a group.

Omit keyword to remove filter.

With this command you can specify two IP Filter files for a given group. You need to specify the allow file first. E. g.:

```
set filter /g=mdl-csd /filter=/xfire/sys/ip/<your-group>.allow,/xfire/sys/ip/<your-group>.deny
```
COMMAND SET ALERT

SET ALERT [/TIME=...] [/HITS=...] [/SETS=...] [/RUN=...] [/EACH=...] [/DATE=...] [/UPDATE=...] [/MAIL=...] [/FROM=...] [/PORT=...] [/IMSG=...] [/YPWD=...] [/NUMAL=...] [/ALUSR=...]

For alerts: max. time (sec), hits/hitsets per order, starting time HHMMSS, run interval (days), prior run date YYYYMMDD, update timestamp FF_YYYYMMDD:HHMMSS, mail server, sender name, SMTP port, initial mail message, mail UID/PWD, max. total alert count, max. alerts per user

This command may be issued with one or more of the optional parameters.

/TIME Defines the maximum duration of a single alert order. Queries running longer are canceled. A value of 0 prevents all alerts from running. Default is 60 seconds.

/HITS Maximum number of hits saved in the permanent hitset created for each alert order. If surpassed for an order, no hits are saved permanently. Default is 10000.

/SETS Number of hitsets per alert order being kept in addition to the one arising on each run. At most SETS+1 hitsets will be kept per alert order. Default is 1.

/RUN Time of day (HHMMSS) when the daily alert processing begins. Default is 000000.

/EACH Run the alert processor each N days, default is 1.

/DATE Date (YYYYMMDD) of the last alert run, set automatically.

/UPDATE Use format FF_YYYYMMDD:HHMMSS to set the time stamp of a database family where FF = BS (Beilstein), GM (Gmelin), or PA (Patents).

/MAIL Name or IP address of the mail server.

/PORT 25 for SMTP, 0 to disable mails being sent.

/FROM Mail address of the person appearing as the sender of automatic mails, user@domain.

/IMSG Initial message sent to the mail server. “EHLO ...” (possibly with parameters) request SMTP extensions, default is HELO (no extensions).
/XMSG User ID for authentication against the mail server. IMSG=EHLO... is required. The alert processor is supporting LOGIN and CRAM-MD5 as authentication methods.

/YMSG Password for the mail server. It is saved in encrypted form, but visible during typing.

/NUMAL Maximum number of alerts processed in the daily run. Additional alerts are skipped. Sequence is alphabetical through user (1) and alert (2) names. Default is 50.

/ALUSR Maximum number of alerts processed per user. Additional ones are skipped. Sequence is alphabetical through alert names. Default is 5.

COMMAND SHOW DATABASES
SHOW DATABASES Show all installed databases.
This will display all available and installed databases:

• A customer database can be used.

• A delivered database can only be used according to the available license.

COMMAND SHOW DUMP
SHOW DUMP [/FILE=<filename>] [ALL]
Show file, def. current dump file. 20 or 10000 lines.
This will display the content of the capture file.

COMMAND SHOW GROUPS
SHOW GROUPS Show all groups.
This will display all groups.

COMMAND SHOW ALERT
SHOW ALERT Show alert parameters.
This will display all alert settings, like mailserver etc.

COMMAND STOP CROSSFIRE
STOP CROSSFIRE Stop the manager and all sessions.
This will terminate the CrossFire system.

Restart:
• AIX: CrossFire daemon reps. batchjob has to be started again

• MS Windows NT: Start the service XFIRED from within the Control Panel or remove the service with „xfired remove“ first and relaunch the CrossFire daemon with „xfired install“.

**COMMAND TEST PERMISSION**

```
TEST PERMISSION  [/GROUP=...] [/PRODUCT=...] /VALUE=...
```

This command may be used to test the access permission for a user name (GROUP and PRODUCT present, VALUE is a user name) or an IP address (PRODUCT is absent, GROUP is present or absent, VALUE is a dotted IP address).

Please refer to chapter Access Filtering for more details on this topic.
### 3.3.7.2.2 Licensing Commands

**COMMAND CLEAR LICENSE**

```
CLEAR LICENSE        [/PRODUCT=...] [/UID=...] [/STATION=...]
[/GROUP=...] [/COUNT=...]: Modify license.
```

This command can only be used if the appropriate license has been installed. The system administrator can use this command to manage named accounts and seat licenses. Related topic: Command Set License

- **Remove a named user**
  
  ```
  [/GROUP=...] /PRODUCT=... /UID=... [/COUNT=...]
  ```

  (a user, which has been entered several times can be removed several times)

- **Remove a registered station with the station ID:**
  
  ```
  [/GROUP=...] /PRODUCT=... /STATION=...
  ```

- **Remove an entire group:**
  
  ```
  /GROUP=...
  ```

- **Remove a specific product within a license group**
  
  ```
  /GROUP=... /PRODUCT=...
  ```

**COMMAND PURGE LICENSE**

```
PURGE LICENSE  [/GROUP=...]
```

This command removes all expired licenses for a group.

**COMMAND REFRESH LICENSE**

```
REFRESH LICENSE  [/GROUP=...]
```

This command will make a new license state available to users. Every change of a license and every manual change of XFIRED.CFG and XFIRE.INI will only be entered into the .LIC files first. The command TRY LICENSE checks whether the modification will cause an error or not. If TRY LICENSE returns no errors, then the command REFRESH LICENSE will activate the changes for the system.

Currently active users will be deactivated and reactivated with the new license information. This fails if the new license is a limitation to a previous license.

This command operates on the licenses of one group only to increase performance. The global refresh was also optimized.
**COMMAND SET LICENSE**

**SET LICENSE** [/LOCALFILE=<filename>] [/KEY=<encoded>] [/PRODUCT=...] [/UID=...] [/STATION=...] [/NAME=...] [/GROUP=...] [/COUNT=...]: Add or update license.

The functions of this command are:

- **Getting product licenses from a license file**
  
  /LOCALFILE=<filename>

  (The license file has to be transferred to the server.)

- **Manual entering of a single product license**
  
  /KEY=<encoded>

  (The encrypted text has to be entered manually.)

- **Adding a named user**

  [/GROUP=...] /PRODUCT=... /UID=... [/COUNT=...]

  (The default setting for GROUP is „DEFAULT“. A user can be entered several times and can log into the system several times. This function requires an appropriate license. Product means the database name, e. g.:PlusAbsPlusEco)

- **Adding a registered station using a station ID and a station name (option). This function should only be used if anything needs to be fixed. The CrossFire client will use it automatically (this function requires an appropriate license).**

  [/GROUP=...] /PRODUCT=... /STATION=... [/NAME=...]

  STATION means the StationID of a Commander Installation and NAME the according StationName.

**COMMAND SHOW LICENSE**

**SHOW LICENSE** [/PRODUCT=...] [/GROUP=...]: Display license.

This display command works in the same manner as the GROUP command.

**COMMAND TRY LICENSE**

**TRY LICENSE**

Every change of a license and every manual change of XFIRED.CFG and XFIRE.INI will only be entered into the .LIC files first. The command TRY LICENSE checks whether the modification will cause an error or not. If TRY LICENSE returns no errors, then the command REFRESH LICENSE will activate the changes for the system.
3.3.7.2.3 Accounting Commands

The CrossFire Accounting System and its commands will only be available if an appropriate license is installed. Please use the command “show license” to check that the product “xfaccounting” is installed. If you do not see this product in the list of installed products then all commands described in this chapter will return the error message “DENIED”.

**COMMAND EXCLUDE COMMAND**

EXCLUDE COMMAND {<command>} : Exclude commands from the log.

This will change the list of commands, which should be accounted. Several commands can be entered if they are divided by a space.

If a command name ends with an underscore then arguments are omitted. Please refer to chapter 3.3.2 The MDL CrossFire Server “xfire” on page 98 for more details on server commands.

**COMMAND GET LOG**

GET LOG (<last> | <all>) : Display the log file contents.

This command will show the last 20 (default) or (at most) 10000 lines.

Will display the content of the accounting log file: the command GET LOG [LAST] will display the first 20 lines, the command GET LOG ALL will display the last 10.000 lines.

**COMMAND INCLUDE COMMAND**

INCLUDE COMMAND {<command>} : Include commands into the log.

This will change the list of commands, which should be accounted. Several commands can be entered if they are divided by a space.

If a command name ends with an underscore then arguments are omitted. Please refer to chapter 3.3.2 The MDL CrossFire Server “xfire” on page 98 for more details on server commands.
**COMMAND NEW LOG**

NEW LOG         Rename the current log file (new name is shown).
Rewrite the current file from its start.

This will rename the accounting log file:

- The name extension of the current log file will be replaced by a number (three digits) or the file number will be added to the file name. The lowest number will be chosen that will lead to a free file name.

- A new log will be initialized with the old name.

**COMMAND SHOW COMMANDS**

SHOW COMMANDS    Show commands being accounted.

This command displays the MDL CrossFire Server commands, which will be stored and monitored during an accounting. If the name of a command ends with an underscore, then only the name of the command is stored and not the parameters of the command.

**COMMAND SHOW LOGNAME**

SHOW LOGNAME     Display the current log file name.

Will display the name of the log file.

**COMMAND START / STOP ACCOUNTING**

Accounting can be applied to one specific license group or to all groups of a server installation.


Start of the accounting: the CrossFire daemon will write all available accounting information into a log file. Only those MDL CrossFire Server which have been used after this command will send accounting information.

STOP ACCOUNTING   [/GROUP=group] : Stop accounting XFire commands.
3.4 The MDL CrossFire Server: Configuration Files

3.4.1 GENERAL
The configuration of the CrossFire system and all licensing information is stored in five different types of files. They are all located in the CrossFire sys directory, e.g.:

- AIX: /xfire/sys
- NT: d:\xfire\sys

Except of the file XFIRE.INI, which is located in the bin directory

- AIX: /xfire/bin
- NT: d:\xfire\bin

of the CrossFire system and the DST files, which can be located anywhere.

All files have the same format like the XFIRE.INI file (except the DST file):

- The content is divided into sections by header lines [Name].

- The sections contain keyword parameters
  KEY=contents;
  which have to be closed by a final semicolon. The system reads all entries up to the semicolon even if line feeds are entered.

- Section header lines and keywords can be written in either capital or small letters.

**Important:** all files described in the following should only be accessible and changeable by the CrossFire administrator. It is not necessary that a normal CrossFire user can even read these files.
3.4.2 THE SERVER CONFIGURATION FILE XFIRE.INI

3.4.2.1 Contents of the CrossFire Configuration File

The CROSSFIRE configuration file xfire.ini is usually maintained only by the xfmaint maintenance program. The following information is given to possibly detect or repair a damaged file.

"xfire.ini" is an ASCII text file. Heading lines of the type

[section_name]

introduce file sections. After the last section, there is a final line containing a single character "["

Sections contain keyword parameters like

keyword_name=value;

Values to keywords are single text strings or comma-separated lists. They may extend over multiple lines. The following table explains all possible keywords:

<table>
<thead>
<tr>
<th>Section</th>
<th>Keyword</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>[CONFIG]</td>
<td>-</td>
<td>Keyword values in this section are maintained by the installation and licensing procedures only.</td>
</tr>
<tr>
<td>[INSTALLATION]</td>
<td>FILESYSTEMS</td>
<td>List of all file systems accommodating new CROSSFIRE database files during installation.</td>
</tr>
<tr>
<td></td>
<td>TAPESIZE</td>
<td>Approximate size of a tape cartridge in bytes.</td>
</tr>
<tr>
<td>[CLIENTDATA]</td>
<td>DBNAMES</td>
<td>Names of the Beilstein, Gmelin or Customer databases currently installed. Each name in the list must also appear as a section heading [database_name].</td>
</tr>
<tr>
<td></td>
<td>DBTOKENS</td>
<td>Same contents as DBNAMES.</td>
</tr>
</tbody>
</table>
| DBSYNTAX       | List of database syntax codes (same number of entries as DBNAMES): Currently always ”1“.
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>DBACCESS</td>
<td>List of database access modes (same number of entries as DBNAMES):</td>
</tr>
<tr>
<td></td>
<td>A  Read/Write access.</td>
</tr>
<tr>
<td></td>
<td>R  Read access.</td>
</tr>
<tr>
<td></td>
<td>N  No access.</td>
</tr>
<tr>
<td></td>
<td>NA Read/Write access, but currently disabled.</td>
</tr>
<tr>
<td></td>
<td>NR Read access, but currently disabled.</td>
</tr>
</tbody>
</table>
| DBMODE         | List of database structure modes (same number of entries as DBNAMES): Currently always ”ORG“.
<p>| CFDIR          | List of data structure table names (same number of entries as DBNAMES): It must be base file names without a path. |
| [database_name]| PACKAGE  Full path name of the package file.                                    |
| DST-&lt;product name&gt; | Full path name of the data structure table for a specific database product. All subsequent parameters except COMMON_INTNAME also have to be (lists of) full path names. This can be a multiple entry e.g.: |
|                | DST_PLUSRXN=/XFIRE/db/xfreas4.dst;                            |
|                | DST_PLUSRXNPLUSABS=/XFIRE/DB/XFABS4.DST ;                           |
| COPYRIGHT      | Full path name of a file containing the copyright statement                     |
| EXPTAB         | Expansion table for compressed structures. Beilstein databases only.            |
| ADD            | Index to the structure display (SDF) file. Beilstein / Gmelin databases only.   |
| SDF            | List of structure display (SDF) files. Beilstein / Gmelin databases only.       |</p>
<table>
<thead>
<tr>
<th>File Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INDEX</td>
<td>Index to structure search files.</td>
</tr>
<tr>
<td>SEARCH</td>
<td>List of structure search files.</td>
</tr>
<tr>
<td>TREE</td>
<td>List of hierarchical index files to structure search files.</td>
</tr>
<tr>
<td>RADD</td>
<td>Index to the reaction display (SDF) file. Beilstein databases only.</td>
</tr>
<tr>
<td>RSDF</td>
<td>List of reaction display (SDF) files. Beilstein databases only.</td>
</tr>
<tr>
<td>RINDEX</td>
<td>Index to reaction search files.</td>
</tr>
<tr>
<td>RSEARCH</td>
<td>List of reaction search files.</td>
</tr>
<tr>
<td>RTREE</td>
<td>List of hierarchical index files to reaction search files.</td>
</tr>
<tr>
<td>JOURCODE</td>
<td>Table of journal titles and CODENs.</td>
</tr>
<tr>
<td>BASE</td>
<td>Common index files to facts, reactions, and citations. Beilstein databases only.</td>
</tr>
<tr>
<td>FACTIDX</td>
<td>Index files to factual data. Beilstein databases only.</td>
</tr>
<tr>
<td>FACTS</td>
<td>Factual data files. Beilstein databases only.</td>
</tr>
<tr>
<td>FACTTTVI</td>
<td>Expansion tables to factual data. Beilstein databases only.</td>
</tr>
<tr>
<td>REACTIDX</td>
<td>Index files to reaction data. Beilstein databases only.</td>
</tr>
<tr>
<td>REACT</td>
<td>Reaction data files. Beilstein databases only.</td>
</tr>
<tr>
<td>REACTTTVI</td>
<td>Expansion tables to reaction data. Beilstein databases only.</td>
</tr>
<tr>
<td>CITATIDX</td>
<td>Index files to citation data. Beilstein databases only.</td>
</tr>
<tr>
<td>CITAT</td>
<td>Citation data files. Beilstein databases only.</td>
</tr>
<tr>
<td>-----------</td>
<td>------------------------------------------------</td>
</tr>
<tr>
<td>CITATTVI</td>
<td>Expansion tables to citation data. Beilstein databases only.</td>
</tr>
<tr>
<td>COMMON_INTNAME</td>
<td>Always containing “CUSTOMER”.</td>
</tr>
<tr>
<td>COMMON_DATA</td>
<td>Customer database data file list.</td>
</tr>
<tr>
<td>COMMON_INDEX</td>
<td>Customer database index file.</td>
</tr>
</tbody>
</table>
3.4.3 THE CROSSFIRE MANAGER CONFIGURATION FILE XFIRED.CFG

This file contains the global settings for the CrossFire daemon and the license groups. The CrossFire administrator can modify it but it is recommended to create a security copy before editing.

Manual changes are only taken into account if the command REFRESH LICENSE is executed from within XFMANAG (see below). It is recommended to use the following method:

- Run XFMANAG and enter the command TRY LICENSE. This makes sure that no errors are entered and all license groups are still known.

- The command REFRESH LICENSE activates all changes.

- If port numbers are changed then the CrossFire daemon XFIRED has to be restarted.

The file XFIRED.CFG contains the following sections:
3.4.3.1 **Section [Manager]**

This section describes the communication of the CrossFire daemon with the daemon control client. It contains the following keywords:

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Port</td>
<td>TCP-Portnumber for the connection to the control client XFMANAG. Default setting is 8004. XFIRED accepts one connection on this port in the maximum and the counterpart needs to run on the same machine. The port numbers in all sections needs to be different.</td>
</tr>
<tr>
<td>UserID</td>
<td>If this keyword has been set only the user with the name mentioned here is allowed to use XFMANAG.</td>
</tr>
<tr>
<td>UserFilter</td>
<td>Complete path to a file that can be used as a filter for usernames. If the previous keyword UserID is empty this list can be used to control the access to the control client. Please see below for details on this file.</td>
</tr>
<tr>
<td>Dumpfile</td>
<td>Complete path to a file that should be used for the protocol of a control client session. Default is <code>&lt;Systemdirectory&gt;/xfmanagelog</code>, e.g. /xfire/sys/xfmanagelog (AIX) d:\xfire\sys\xfmanagelog (NT)</td>
</tr>
<tr>
<td>DoDump</td>
<td>Content ON or OFF: Switch for activating or deactivating the session protocol. Default setting is OFF.</td>
</tr>
</tbody>
</table>
3.4.3.2 **Section [CrossFire]**

Contents: parameter of the communication between MDL CrossFire Commander (CrossFire client) and the CrossFire daemon XFIRED.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Port</td>
<td>TCP port which is used for getting a connection to the CrossFire client (MDL CrossFire Commander). Default is 8001. The CrossFire daemon starts a dispatcher and hands over the communication to it.</td>
</tr>
</tbody>
</table>
| Program     | Pathname, from which the MDL CrossFire Server should be loaded. Default is the BIN directory parallel to the directory, which contains the XFIRED (.EXE), e.g.  

```
/xfire/bin  if xfiRed is in /xfire/sys.
```

| RootPath    | Name of the path to the subdirectories USR and TMP of a CrossFire installation. Default is the root directory to the directory, which contains XFIRED, e.g.  

```
/xfire  if xfiRed is in /xfire/sys.
```

A similar expression should be entered for every license group. The existence of this entry for every license group is essential, if Telnet is used.

| Filter      | Complete path to a file, which contains IP addresses of clients, which are allowed to run CrossFire (please refer to sections below on the contents of this file). If this entry is missing every IP address is accepted. |
### 3.4.3.3 Section [Accounting]
Content: setting for controlling the accounting feature of the CrossFire feature. The keywords Account...= should not be edited manually. Use XFMANAG instead.

<table>
<thead>
<tr>
<th>Port</th>
<th>TCP port which should be used for sending accounting information to. Default is 8002.</th>
</tr>
</thead>
<tbody>
<tr>
<td>AccountCommands</td>
<td>Comma separated list of MDL CrossFire Server commands, which should be sent by the MDL CrossFire Servers.</td>
</tr>
<tr>
<td>AccountLog</td>
<td>Complete path to the accounting log file. Default is &lt;CrossFire sys directory&gt;/xfacct.log</td>
</tr>
</tbody>
</table>

### 3.4.3.4 Section [Licensing]
Content: Settings for licensing

<table>
<thead>
<tr>
<th>Port</th>
<th>TCP port for the internal communication between MDL CrossFire Servers, CrossFire dispatchers and the CrossFire daemon. Default is 8003.</th>
</tr>
</thead>
<tbody>
<tr>
<td>RegClient</td>
<td>ON or OFF: CrossFire clients will be enabled to use the command „Register Station“. Default is ON. This is only valid, if the license is set to „seat“ licensing.</td>
</tr>
<tr>
<td>RegUser</td>
<td>If this parameter is set then a CrossFire client has to log into the system with this name after a successful „Register Station“.</td>
</tr>
<tr>
<td>Master</td>
<td>IP Address of the Master Server, current machine is the Slave. This only applies if at least two MDL CrossFire Server run as a Master-Slave System.</td>
</tr>
<tr>
<td>Slaves</td>
<td>IP Address of the Slave Servers, current machine is the Master. This only applies if at least two MDL CrossFire Server run as a Master-Slave System.</td>
</tr>
</tbody>
</table>
### 3.4.3.5 Sections [Group-Group name]

Each license group of an installation needs to have this entry with the name of the group. If this entry is deleted the group can no longer use the system.

Optional parameters are:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>RootPath</strong></td>
<td>If this parameter has been set then it supersedes the setting in section [CrossFire] for this group.</td>
</tr>
<tr>
<td></td>
<td>Setting or not setting of this parameter has the following result:</td>
</tr>
<tr>
<td></td>
<td>• If this parameter has been set then „old“ clients are assigned to the current group, if the parameters in the client have been set appropriately (Options/Connections: CrossFire root directory).</td>
</tr>
<tr>
<td></td>
<td>• Customer databases are only available if this parameter has been set. There need to be a BIN directory in this root path, which contains a XFIRE.INI file. The customer database has to be defined in the XFIRE.INI file.</td>
</tr>
<tr>
<td><strong>UserFilter</strong></td>
<td>Complete path to a file, which allows or denies the access of users with a specific name, if a license has been set to „concurrent“ usage.</td>
</tr>
<tr>
<td><strong>Accounting</strong></td>
<td>ON or OFF: switch that controls the accounting. A missing entry means OFF.</td>
</tr>
<tr>
<td><strong>TimeOut</strong></td>
<td>0 is the default and will let the server shutdown after 2h of inactivity. The timeout can be set in seconds.</td>
</tr>
<tr>
<td><strong>UserDir</strong></td>
<td>Complete path to a directory, where the MDL CrossFire Server can create user directories. User directories will be used for storing temporary and permanent hitsets.</td>
</tr>
<tr>
<td><strong>TempDir</strong></td>
<td>Complete path to a directory that can be used by the MDL CrossFire Server for writing temporary files.</td>
</tr>
</tbody>
</table>
Example:

[Manager]
PORT=8004;
USERID=xfadmin;
DumpFile=/xfire/sys/xfmanage.log;
DoDump=OFF;
UserFilter=/xfire/sys/ctrl.flt;

[CrossFire]
Port=8001;
Program=/xfire/bin;
RootPath=/xfire;
Filter=/xfire/sys/ip.flt;

[Accounting]
Port=8002;
AccountCommands=search,,,send,,,dbselect,init,exit;
AccountLog=/xfire/sys/xfacct.log;

[Licensing]
Port=8003;
RegUser=xfadmin;

[Group-GRP1]
RootPath=/xfire/;
Accounting=ON;
UserDir=;
TempDir=;
TimeOut=0;
UserFilter=;
### 3.4.4 LICENSE FILES (EXTENSION .LIC AND .XFL)

#### 3.4.4.1 Group License File <Group name>.LIC

Single product licenses of a CrossFire installation are assigned to one or more license groups. Every license group gets a file `<groupname.lic>` that is located in the SYS directory of the CrossFire installation. These files cannot be edited manually. Any manual change of these files corrupts them and the group can no longer use CrossFire. They contain the following entries:

<table>
<thead>
<tr>
<th>Section</th>
<th>Keyword</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>General</td>
<td>Signature</td>
<td>File security key</td>
</tr>
</tbody>
</table>
| License       | Product name| This section contains one keyword parameter for every product that is licensed for a specific group. The structure is as follows:  
Encoded license parameter, comma, comment |
| Product name  | UserNo.     | For every product the names of licensed users have to be entered under the title of the product. Keywords are User1, User2, ... |
| Product name  | StationNo.  | In the same section you will see the code and name of registered stations. The contents for the keywords Station1, Station2, ... are:  
Station-ID, comma, Station name (optional). |
Example:

[General]
Signature=3HQ200IINHL5NO9IKOINTOAENDKBA4B71QKCAR91L5NGLVNO0NVOMNT1DK1A
UB41DKOA3;

[License]
Gmelin=3TC6POII69ETH88FSU1P2R01SP1SC5N6J5C4R52S1G0SNUN69PO468P4UTV3GH6E5
8TVMRKS1PNRAV9UDVAUS6M86A8H6986E6L8G6LUN3FUN3F77SCRJ3F,Date:2005.04.22,Conc:999,Named:0,Sites:0;

PlusAbsPlusEco=UBP2HUIII8FGAPC6L524RHS357RHR78F48EF8U1FS7RE574448FHUUQ6IUO
VKRMPQG06ATG37.0R506IT56LVARMET6L5N475OUQPRM574SB74SD78SN76SNRL47RL478F
6JUC47,Date:2005.04.22,Conc:999,Named:0,Sites:0;

XfAccounting=ROVI8PIIIH7UB6JPNROEV85FSTV8VTE3HH83EGK35TV4STHEHH78PGMPQGIS1
5Q6MU2P76FRTVU2PSC50CGI35H4SCGLS25CVJTPVKTPVOIVITEVI50FRTVVI50FR,Date:
2005.04.22,Conc:0,Named:0,Sites:0;

XfEncryption=UNVI0MII1BA79HB8LV200KQ10000OLIJI1NILD5IK00K1OJ2J1B0MDP6DGJS
CU9PAB7MOQ020AR3J7DF9E0IJS1QJUDGJ4D5BS1BB41B81BI32B32DT2L1NB3DT2L,Date:
2005.04.22,Conc:0,Named:0,Sites:0;

XfExportAll=GKC80MIIERA79HB8LV200KQ10000OLIJI1NILD5IK00K1OJ2J1B0MDP6DGJS
CU9PAB7MOQ020AR3J7OA9HC6KNCA7ANFA79F09K9G09V09VARK10K9PAUK1,Date:20
05.04.22,Conc:1,Named:0,Sites:0;

XfRxnSearch=5CC8NTIIJ6Q0O0M12LHLNEA89HHN95DJV5SD5LDE9HC89VLCJ6N19MBIA1NK
DO9QCMOB7A49QCMQC4J11A8BB43Q2MB2J1CBU11B0B16B02IDVBR12IDV,Date:20
05.04.22,Conc:0,Named:0,Sites:0;

XfStrSearch=H8C8NTIIJ6Q0O0M12LHLNEA89HHN95DJV5SD5LDE9HC89VLCJ6N19MBIA1NK
DO9QCMOB7A49QCMQC3KDCRMQNMBSA3NEC8QOCRQOCSQCUQCCUNP0KQ1CUNPOK,Date:20
05.04.22,Conc:0,Named:0,Sites:0;

[Gmelin]

[PlusAbsPlusEco]

[XfAccounting]

[XfEncryption]

[XfRxnSearch]

[XfStrSearch]
### 3.4.4.2 License File `<name>.XFL`

The first or modified licenses are delivered in a file that has the following structure:

<table>
<thead>
<tr>
<th>Section</th>
<th>Keyword</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Group name</strong></td>
<td><strong>Product name</strong></td>
<td>The content of a keyword, which belongs to a product is built in the same way like in the group license file:</td>
</tr>
<tr>
<td><strong>Enc</strong></td>
<td><strong>Dec</strong></td>
<td><strong>Comment</strong></td>
</tr>
</tbody>
</table>

**Example:**

```
[your-group]
Gmelin=3TC6POII69ETH88HFSU1P2R0S1P1SC5N6J5C4R52S1G0SNUN69PO468P4UTV3GH6E5
8TVMRKS1PNRAV9UDVAUQ6M8H6A8H698E6L8G6LUN3FUN3F77SCRJ3F,Date: 2005.04.22,Conc: 999,Named: 0,Sites: 0;
PlusAbsPlusEco=UBP2HUII8FGAPC6L524RHS357RHR78F48EF8U1FS7RE574448FUUQ6IUO
VKRMPQG06ATG37.0R506IT56LVARMET6L5N475OUQPNRMSQ74SB74SD78SN76SNRL47RL478F
6JUC47,Date: 2005.04.22,Conc: 999,Named: 0,Sites: 0;
XfAccounting=R0V18PIIIH7UB6JPNRQEV85FSTV8VTE3HH83EGK35Tv4STHEHH78PGMPOGIS1
5Q6MU2PB76FRTVU2PDSC5OSCGIHOH4SCGLS25CVJTPVKTPV9GIVVEI50FRTV5I5FR,Date:
2005.04.22,Conc: 0,Named: 0,Sites: 0;
XfEncryption=UNVI0MI11B79HB8LV200KQ1000000LIJ1NILD5IK0K08J2J21BOMDP6BGJS
CU9PARB7MQQ200ARB3J7DP9EOIJS1QJUDGJ4D5S1BB41BB81DB312B3DT2L1NB3DT2L,Date:
2005.04.22,Conc: 0,Named: 0,Sites: 0;
XfExportAll=GC80MI11B79HB8LV200KQ1000000LIJ1NILD5IK0K08J2J21BOMDP6BGJS
CU9PARB7MQQ200ARB3J70A9HC6KNC8ATF879F0K90G09V099VARK10K9PAUK1,Date:
2005.04.22,Conc: 1,Named: 0,Sites: 0;
XfRxnSearch=5CC8NTIIJ6Q000M12JLHNEA89HH95DVJSD5ILDE9HC89VLVJ6NTI9MBIA1NK
DO9QCMOB7A49HQC8M4C4J11BA3A9Q2MB2J1CBUI1BU12B61OB81O2IDV8R102IDV,Date:
2005.04.22,Conc: 0,Named: 0,Sites: 0;
XfStrSearch=H8C8NTIIJ6Q000M12JLHNEA89HH95DVJSD5ILDE9HC89VLVJ6NTI9MBIA1NK
DO9QCMOB7A49HQC8M4C3KDRCMCQNMBSA3NEC8QOCRQOSQQCUCUNP0K1CUNP0K,Date:
2005.04.22,Conc: 0,Named: 0,Sites: 0;
```
3.4.5 ACCESS FILTERING
It is possible to restrict the access to the MDL CrossFire Server by defining various access filters. This chapter describes how to create and use IP filters and user filters.

Filters may be installed at the following locations in file xfired.cfg, instead of manually editing the xfired.cfg we recommend to specify a filter file with xfmanag:

<table>
<thead>
<tr>
<th>Section/Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Manager]</td>
<td></td>
</tr>
<tr>
<td>UserFilter=filename</td>
<td>users permitted to specify commands towards the XFIRE daemon using xfmanag</td>
</tr>
<tr>
<td>[CrossFire]</td>
<td></td>
</tr>
<tr>
<td>Filter=pair_of_filenames</td>
<td>Comma-separated list of path and file names of files containing the TCP/IP addresses permitted/denied to connect to the XFIRE port (e.g. \xfire\sys\hosts.allow, \xfire\sys\hosts.deny)</td>
</tr>
<tr>
<td>[Group-groupname]</td>
<td></td>
</tr>
<tr>
<td>UserFilter=filename</td>
<td>Users permitted to add load to a CONCURRENT license of a specific product available to a group. Other license types are not concerned.</td>
</tr>
<tr>
<td>Filter=pair_of_filenames</td>
<td>Comma-separated list of paths and files names of files containing the TCP/IP addresses permitted/denied to connect to the XFIRE port (e.g. \xfire\sys\hosts.allow, \xfire\sys\hosts.deny). Valid for the current group when making a connection to the XFIRE port.</td>
</tr>
</tbody>
</table>
3.4.5.1 **IP Address Filtering**

For an IP address filter, a comma-separated pair of 2 file names (permit file, deny file, e.g. `\xfire\sys\hosts.allow,\xfire\sys\hosts.deny`) has to be specified.

Lines starting with a hash mark are ignored. Other lines are evaluated if they contain one or two colons plus a substring “xfire” (quotes not within the line) before the first or only colon.

IP address filters can be installed for an entire CrossFire installation or for each installed license group separately.

The line section between the first and second colon or end of line has to contain items separated by blanks or commas. Possible items and their meaning are:

<table>
<thead>
<tr>
<th>IP address</th>
<th>#.#.#.#, each # is a number 0-255. Matched exactly against the IP address of a connection.</th>
</tr>
</thead>
<tbody>
<tr>
<td>right-truncated IP address</td>
<td>{#.}, i.e. 1 to 3 repetitions of # + dot. Matches any IP address starting with these 1 to 3 numbers.</td>
</tr>
<tr>
<td>IP ranges</td>
<td>#.#.#.x-y, each # is a number 0-255. Matched exactly against the IP address of a connection. x and y define the lower and upper limit of an IP range.</td>
</tr>
<tr>
<td>IP address and mask</td>
<td>value/mask where value and mask look like &quot;#.#.#.#&quot;. An IP address matches if (adr &amp; mask) == value.</td>
</tr>
<tr>
<td>host name</td>
<td>An IP address matches if it gets that host name assigned by name server address resolution. An irresolvable address receives an empty name.</td>
</tr>
<tr>
<td>left-truncated host name</td>
<td>String starting with a dot. An IP address matches if its corresponding host name ends with that string.</td>
</tr>
<tr>
<td>word ALL</td>
<td>Any IP address</td>
</tr>
<tr>
<td>word KNOWN</td>
<td>Any IP address receiving a non-empty host name.</td>
</tr>
<tr>
<td>word UNKNOWN</td>
<td>Any unresolvable IP address.</td>
</tr>
<tr>
<td>word LOCAL</td>
<td>Any resolvable address with a host name containing no dots.</td>
</tr>
<tr>
<td>word PARANOID</td>
<td>Any address which is not resolvable or whose host name either yields no hit on name resolution or yields a different address.</td>
</tr>
</tbody>
</table>
word EXCEPT

<table>
<thead>
<tr>
<th>word EXCEPT</th>
<th>After the word EXCEPT, the consequences of a match are inverted for the subsequent items:</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) If the item resides in the allow file and is matched, the matching IP address is rejected.</td>
<td></td>
</tr>
<tr>
<td>2) If the item resides in the deny file and is matched, the IP address is accepted if there is no withstanding prior match.</td>
<td></td>
</tr>
</tbody>
</table>

Items with EXCEPT in the allow file are collected in an "except" list, items without in an "allow" list. Items with EXCEPT in the deny file are appended to the "allow" list, items without are added to a "deny" list, in each case maintaining the input sequence or items.

An incoming IP address is matched against the except list, the allow list and finally the deny list. On the first match, it is rejected (except and deny list), or accepted.

When no match at all occurs, it is accepted.

The command TEST PERMISSION [/GROUP=...] [/PRODUCT=...] /VALUE=... may be used to test the access permission for a user name (GROUP and PRODUCT present, VALUE is a user name) or an IP address (PRODUCT is absent, GROUP is present or absent, VALUE is a dotted IP address).

Example:

Allow File

```
# allowed addresses for group <yourgroup>
xfire:172.31.,172.17.,10.0.
xfire:169.102.
xfire:172.17.28.0-172.18.255.255
```

Deny File

```
# denied addresses for group <yourgroup>
xfire:ALL
```

### 3.4.5.2 User Name Filtering

In XFIRED.CFG two types of user filters can be entered:

- **Section [Manager], Keyword UserFilter**: This filter has to be activated through XFMANAG and will ensure that only those users listed in the filter file will
be able to use XFMANAG. The file is structured like an IP address filter file. Instead of IP addresses usernames or an asterisk for „every user“ is used.

• **Section** [Group-Group name], **Keyword** UserFilter: a concurrent user is able to use a specific product in a specific group.

User filter files should start with a heading [product_name] to name the product referred to. Beneath, user names or name masks have to be specified as values in one or more of the following keyword parameters:
EXCEPT=...;

PERMIT=...;

DENY=...;

The syntax is “KEYWORD equal_sign value semicolon”. Line feeds may intervene, blanks may not. The value may be a single item or a comma separated list of items.

Items are:

a. User name (matched ignoring case).

b. A mask with an appended asterisk for right truncation.

c. An asterisk for "all users".

The keywords may occur in any order in the filter file. However, there is an order in how CrossFire applies the filter criteria. A user name is matched at first against all EXCEPT values or masks followed by all PERMIT values and finally all DENY values. On the first match, access is permitted or denied (for EXCEPT and DENY). If no match occurs, access is permitted.

Example:

[product1]          # for Product1:
except=xfuser1;     # xfuser1 is not a concurrent user.
permit=*

[product2]          # for Product2:
permit=xfuser2;     # only xfuser2 is a concurrent user.
deny=*;

With this example a user "xfuser1" will not be able to use product1 but all other users. "xfuser2" will be able to use product2 but nobody else.

The following filter would NOT work as expected (= to deny access for user "xfuser1"):

[product1]          # for Product1:
deny=xfuser1;
permit=*

The MDL CrossFire Server re-orders the filters and will use the PERMIT filter before the DENY filter. As PERMIT allows everybody the DENY filter is not used any more. Only an EXCEPT filter statement would solve this (see example above).
### 3.4.6 BEILSTEIN / GMELIN DATA STRUCTURE TABLE (DST) FILES

#### 3.4.6.1 General Information

The data structure of a Beilstein / Gmelin or Customer database is described in a DST file. It is an ASCII file of sections headed by a `[NAME]` line. Apart from section headings, there are empty (blank) lines, comment lines starting with `//`, and data lines which in most cases are separated into columns using the `|` character.

The following sections will appear:

<table>
<thead>
<tr>
<th>Section</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>[POSITIONS]</td>
<td>The POSITIONS section renders a directory of all data columns in the later sections. It is a table of two columns:</td>
</tr>
<tr>
<td></td>
<td>1. section name</td>
</tr>
<tr>
<td></td>
<td>2. column name</td>
</tr>
<tr>
<td></td>
<td>Lines to a common section have the same order as the data columns in that section (left to right).</td>
</tr>
<tr>
<td>[GENERAL]</td>
<td>The GENERAL section does not contain single data lines, but a data block with keyword parameters</td>
</tr>
<tr>
<td></td>
<td>[keyword=value];</td>
</tr>
<tr>
<td></td>
<td>Keywords include the VERSION value of the file. The CROSSFIRE client programs only use other keywords.</td>
</tr>
<tr>
<td></td>
<td>The keyword SIGNATURE contains an encrypted string that is used for protecting a DST file against unpermitted changes.</td>
</tr>
<tr>
<td>[FILES]</td>
<td>The FILES section has one line per available database context. The first column is the context number, the second the context name.</td>
</tr>
<tr>
<td>[COUPLEINDEX]</td>
<td>The current section defines all context relationships or couplings as pairs of contexts:</td>
</tr>
<tr>
<td></td>
<td>column 1: number of the coupling, 1 to N</td>
</tr>
<tr>
<td></td>
<td>column 2: source file (context): For the current coupling, the file where data fields reside containing ID numbers of a different context.</td>
</tr>
<tr>
<td></td>
<td>column 3: target file. The file whose ID numbers are referenced in fields of the source file.</td>
</tr>
<tr>
<td>Col.</td>
<td>Name</td>
</tr>
<tr>
<td>------</td>
<td>------------</td>
</tr>
<tr>
<td>1</td>
<td>ICODE</td>
</tr>
<tr>
<td>2</td>
<td>TITUPPER</td>
</tr>
<tr>
<td>3</td>
<td>ROWNUMBER</td>
</tr>
<tr>
<td>4</td>
<td>SEARCHABLE</td>
</tr>
<tr>
<td>5</td>
<td>FACTNAME</td>
</tr>
</tbody>
</table>
### Section Facts

<table>
<thead>
<tr>
<th>Col.</th>
<th>Name</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PHYSFILE</td>
<td>Number of the file (context) the property belongs to. Must not be blank.</td>
</tr>
<tr>
<td>2</td>
<td>ICODE</td>
<td>3-character name of a property. This name has to be used in queries with search format. The third character should be an underscore instead of a point in all commands to and data from the server. Must not be blank.</td>
</tr>
<tr>
<td>3</td>
<td>TITUPPER</td>
<td>3-character name of the parent search term or blank for a top-level property.</td>
</tr>
<tr>
<td>4</td>
<td>ROWNUMBER</td>
<td>Row to display the current property in the CROSSFIRE client programs. If blank then this is a non-display fact.</td>
</tr>
<tr>
<td>5</td>
<td>SEARCHABLE</td>
<td>S: Items are searchable for existence of the current property. If blank then this fact cannot be searched in a field availability search.</td>
</tr>
<tr>
<td>6</td>
<td>NONDISPLAY</td>
<td>Y: the CROSSFIRE client does not display the property. If blank then it will be displayed.</td>
</tr>
<tr>
<td>7</td>
<td>FACTNAME2</td>
<td>Short name of the property to be used in display format queries. Must not be blank.</td>
</tr>
<tr>
<td>8</td>
<td>ENAME</td>
<td>Long name of the property. Must not be blank.</td>
</tr>
<tr>
<td>9</td>
<td>TABINFO</td>
<td>Information how the CROSSFIRE client should display a table for the current property. Missing or blank for non-tabular properties.</td>
</tr>
</tbody>
</table>
### Section Fields

<table>
<thead>
<tr>
<th>Col.</th>
<th>Name</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PHYSFILE</td>
<td>Number of the file (context) the field belongs to. Must not be blank.</td>
</tr>
<tr>
<td>2</td>
<td>ICODE</td>
<td>3-character name of a field. This name has to be used in queries with search format. Must not be blank.</td>
</tr>
<tr>
<td>3</td>
<td>ICODEFACT</td>
<td>3-character name of the parent property. Must not be blank.</td>
</tr>
<tr>
<td>4</td>
<td>DISPLAYMODE</td>
<td>N  not displayed</td>
</tr>
<tr>
<td></td>
<td></td>
<td>F  fixed-point number</td>
</tr>
<tr>
<td></td>
<td></td>
<td>I  integer number</td>
</tr>
<tr>
<td></td>
<td></td>
<td>A  field contents is appended to the predecessor field</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Blank  no special action</td>
</tr>
<tr>
<td>5</td>
<td>SEARCHABLE</td>
<td>S  searchable as string</td>
</tr>
<tr>
<td></td>
<td></td>
<td>I  searchable as number (integer)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>R  searchable as number (range)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Blank  not searchable</td>
</tr>
<tr>
<td>6</td>
<td>INDEXING</td>
<td>B  indexed as Boolean value “YES”</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N  numeric</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P  full phrase (for texts)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>R  numeric range. A query interval matches if it overlaps with a data interval.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>W  wordwise (for texts)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Y  wordwise with alternate separator set</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Z  separated at semicolons (for citation authors)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Blank  not indexed</td>
</tr>
<tr>
<td></td>
<td>FUNCTION</td>
<td>Description</td>
</tr>
<tr>
<td>---</td>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>7</td>
<td>P</td>
<td>primary key of the current file</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>comment field</td>
</tr>
<tr>
<td></td>
<td>K</td>
<td>reference field containing an ID number of a different context identified in the REFFILE column. Blank no special function</td>
</tr>
<tr>
<td>8</td>
<td>REFFILE</td>
<td>Target context of a reference field - FUNCTION K (see Col. 7), or zero or blank.</td>
</tr>
<tr>
<td>9</td>
<td>FIELDNAME2</td>
<td>Short field name to be used in display format queries. Must not be blank.</td>
</tr>
<tr>
<td>10</td>
<td>UNITTEXT</td>
<td>Physical unit of the field or blank.</td>
</tr>
<tr>
<td>11</td>
<td>ENAME</td>
<td>Long field name. Must not be blank.</td>
</tr>
<tr>
<td>12</td>
<td>OPTIONS</td>
<td>Search and display options to be interpreted by the CROSSFIRE client programs:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>DH=CVNAME; Field should be displayed as chemical name</td>
</tr>
<tr>
<td></td>
<td></td>
<td>DH=CVSUFO; Display as molecular formula</td>
</tr>
<tr>
<td></td>
<td></td>
<td>DH=SHDISP; Use field in short display.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FE=ELC; Format as element count search field</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FE=MF; Molecular formula search field.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FE=MOFO; General formula search field</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FMT=CN; Format as chemical name</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FMT=CONC; Concatenate field to predecessor</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HYPL=BRN; Hyperlink field using BRN</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HYPL=LBRN; Hyperlink field using BRNs of reactants</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HYPL=RBRN; Hyperlink field using BRNs of reaction products</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HYPL=REACT; Hyperlink field using the reaction ID number</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TYP=CIT; Reference field to a citation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TYP=COM; Comment field</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MULTI=M; field may occur multiple times</td>
</tr>
<tr>
<td></td>
<td>MULTI=&lt;number&gt;; fields with the same number build a repeating group and will appear at the same time one after the other (e.g. Product BRN and Product Name). It is possible that a fact contains several repeating groups.</td>
<td></td>
</tr>
</tbody>
</table>
3.5 The MDL CrossFire Server: Protocol and Log Files

3.5.1 GENERAL

If anything fails during the start procedure of the CrossFire daemon or XFMANAG they will write diagnose files. A description of the contents of these files is given below.

The files XFM...LOG, XFD...LOG, XFS...LOG and XLL...LOG always contain the process number as part of their names. They are only created if an error occurs during the start of the CrossFire daemon, the CrossFire dispatcher or the MDL CrossFire Server.

3.5.2 MESSAGES OF THE CROSSFIRE MANAGER: XFM...LOG

<table>
<thead>
<tr>
<th>Error Message</th>
<th>Possible Reason</th>
</tr>
</thead>
<tbody>
<tr>
<td>XFIRED already running</td>
<td>The CrossFire daemon is already running.</td>
</tr>
<tr>
<td>Cannot open SC manager:</td>
<td>MS Windows NT: no rights for changing entries in the service database.</td>
</tr>
<tr>
<td>Cannot start XFIRED:</td>
<td>MS Windows NT: Error after a successful installation and an attempt to start the service.</td>
</tr>
<tr>
<td>error starting the CTRL dispatcher</td>
<td>MS Windows NT: internal error</td>
</tr>
<tr>
<td>error removing the service:</td>
<td>MS Windows NT: service has been stopped or removed already.</td>
</tr>
<tr>
<td>cannot load:</td>
<td>The file named after the colon cannot be loaded:</td>
</tr>
<tr>
<td>load error:</td>
<td>• Name or Path is invalid, no sufficient rights.</td>
</tr>
<tr>
<td></td>
<td>• Invalid content. In this case detailed error messages are given above.</td>
</tr>
<tr>
<td>Error Message</td>
<td>Description</td>
</tr>
<tr>
<td>---------------</td>
<td>-------------</td>
</tr>
<tr>
<td>ERROR listening on ...</td>
<td>The CrossFire daemon was not able to use the designated port as listener.</td>
</tr>
<tr>
<td>1. Port number is invalid or reserved (&lt; 1024).</td>
<td></td>
</tr>
<tr>
<td>2. A CrossFire daemon run has been stopped right before trying to launch it again. Wait a minute and try it again.</td>
<td></td>
</tr>
<tr>
<td>ERROR create:</td>
<td>AIX and MS Windows NT: The CrossFire daemon was not able to launch a dispatcher for a CrossFire client. File name (may be wrong) and reason is given in the next line.</td>
</tr>
<tr>
<td>CFG file init error</td>
<td>XFIRED.CFG did not exist and could not be created.</td>
</tr>
<tr>
<td>bad program path</td>
<td>Internal error, which should not appear.</td>
</tr>
<tr>
<td>bad root path</td>
<td></td>
</tr>
<tr>
<td>bad accounting log name</td>
<td></td>
</tr>
<tr>
<td>too many databases</td>
<td></td>
</tr>
<tr>
<td>no delimiter ] after [</td>
<td>Format error in file XFIRED.CFG. Correct the error and try it again.</td>
</tr>
<tr>
<td>error creating group</td>
<td>A license group could not be read from a &lt;group name&gt;.lic file. Details should be available from messages, which has appeared previously.</td>
</tr>
<tr>
<td>multiple installation names</td>
<td>Changing product name within different licenses.</td>
</tr>
<tr>
<td>keyword not found:</td>
<td>Internal format error in group license file: the content is not valid.</td>
</tr>
<tr>
<td>invalid signature</td>
<td></td>
</tr>
<tr>
<td>format error for:</td>
<td></td>
</tr>
<tr>
<td>short name not found:</td>
<td></td>
</tr>
<tr>
<td>too many databases</td>
<td></td>
</tr>
<tr>
<td>Issue Description</td>
<td>Error Description</td>
</tr>
<tr>
<td>----------------------------------------------------------------------------------</td>
<td>-----------------------------------------------------------------------------------</td>
</tr>
</tbody>
</table>
| invalid encryption string for product  
invalid encryption key for product  
group name mismatch:  
installation name mismatch: | Erroneous encoding in group license file.                                           |
| no ; after User/Station  
too many users  
station reoccurs:  
too many stations | Erroneous entry for named users or stations. The content of a group license file is invalid. |
| station would exceed maximum:  
user would exceed maximum: | Warning (no error): named users or stations may not be accepted any longer if their number exceeds the limits of a new license. |
| no ; after DST  
product name invalid for DST  
cannot retrieve the product short name | The DST file for a database product is invalid or not accessible:  
  - The parameter in section [CrossFire] RootPath= does not point to the directory which containsXFIRE.INI.  
  - The database defined in XFIRE.INI does not have a DST entry for the current product.  
  - XFIRE.INI contains a wrong file name or points to an invalid file. |
### 3.5.3 MESSAGES OF THE CROSSFIRE DISPATCHER: XFD...LOG

<table>
<thead>
<tr>
<th>Error Message</th>
<th>Possible Reason</th>
</tr>
</thead>
<tbody>
<tr>
<td>Timeout</td>
<td>No answer from a CrossFire daemon or the CrossFire clients within 30 sec.</td>
</tr>
<tr>
<td>/F encryption not supported</td>
<td>Encryption of the Internet communication is not supported or the client has tried to run an invalid command.</td>
</tr>
<tr>
<td>/F bad encryption request</td>
<td>No answer from the CrossFire daemon, i.e. it is not running.</td>
</tr>
<tr>
<td>no response from</td>
<td>A request to the CrossFire daemon has been rejected.</td>
</tr>
<tr>
<td>request denied:</td>
<td>The user of a CrossFire client has used an invalid user name or password or the authentication process has failed for other reasons.</td>
</tr>
<tr>
<td>authorization failure, program:</td>
<td>If the password has been expired the sentence &quot;; password expired&quot; will be added to this message.</td>
</tr>
<tr>
<td>expired</td>
<td>No communication possible with the MDL CrossFire Server.</td>
</tr>
<tr>
<td>server did not connect up</td>
<td>The started MDL CrossFire Server did not respond within 30 sec., i.e. has been terminated unusually.</td>
</tr>
<tr>
<td>exec failed:</td>
<td>The MDL CrossFire Server could not be started. (program name is displayed).</td>
</tr>
<tr>
<td>create process failed</td>
<td>No answer from the CrossFire daemon, i.e. it is not running.</td>
</tr>
</tbody>
</table>
### 3.5.4 Messages of the MDL CrossFire Server: XFS...LOG

<table>
<thead>
<tr>
<th>Error Message</th>
<th>Possible Reason</th>
</tr>
</thead>
<tbody>
<tr>
<td>connect up failed to port:</td>
<td>The MDL CrossFire Server is not able to establish a connection to the dispatcher.</td>
</tr>
</tbody>
</table>

### 3.5.5 Messages of the Socket Communication: XLL...LOG

<table>
<thead>
<tr>
<th>Error Message</th>
<th>Possible Reason</th>
</tr>
</thead>
<tbody>
<tr>
<td>***ERROR: socket() failed!</td>
<td>The respective call to the socket interface failed:</td>
</tr>
<tr>
<td>***ERROR: SetNoInherit() failed!</td>
<td>- The TCP ports used from the CrossFire daemon are reserved or used by other processes: check the port numbers.</td>
</tr>
<tr>
<td>***ERROR: bind() failed!</td>
<td>- If the CrossFire daemon has been stopped and one tries to relaunch it immediately after this, ports may be locked. Wait approx. 1 minute and try it again.</td>
</tr>
<tr>
<td>***ERROR: listen() failed!</td>
<td>- A client program has used a wrong hostname, ip address or port number to get in touch with the CrossFire daemon or the daemon is not running any longer.</td>
</tr>
<tr>
<td>accept error</td>
<td></td>
</tr>
<tr>
<td>too many sockets</td>
<td></td>
</tr>
<tr>
<td>inet_addr() failed!</td>
<td></td>
</tr>
<tr>
<td>***ERROR: close socket due to error!</td>
<td></td>
</tr>
<tr>
<td>non-local:</td>
<td>The ports for licensing, accounting and managing the CrossFire system can only be used locally..</td>
</tr>
<tr>
<td>create ERROR: ...</td>
<td></td>
</tr>
<tr>
<td>ERROR action=...</td>
<td>The CrossFire dispatcher or server (the call is displayed) could not be launched.</td>
</tr>
</tbody>
</table>
3.5.6 FILE XFIRED.MON

This file is used for checking the system clock. If this file is missing the CrossFire daemon will be terminated automatically with the following error message:

    system time check failed

If this happens then the system can be restarted again using two different possibilities:

- If no licenses have been entered this file is created if the CrossFire daemon is launched.

In all other cases any valid license has to be entered within 30 seconds after the system has been started.

3.5.7 FILE VERIFY.LOG / VERIFY.ERR

The file VERIFY.LOG is an ASCII file that contains a session protocol of XFMAINT. Any text editor can read it and it can be browsed in order to get an overview of what have been done in a session.

The file VERIFY.ERR is an ASCII file as well, but instead of having all of the session logged it only contains errors that may have occurred during a database check.

Both files will be located in the CrossFire „sys“ directory.
3.5.8 USER CONFIGURATION FILE <USER NAME>.XFU

Each user with write access to one or more customer databases has a configuration file assigned which defines a set of files for each of these databases. For each database there is a section headed by the database name enclosed in brackets - as for the xfire.ini file. User configuration files also reside in the directory

< CROSSFIRE root > /bin

Keywords in each of the ["database"] sections are:

- **RN_MIN, RN_MAX**
  Minimum and maximum Customer RegNo available for updates by the user.

- **SEQNOS_USER**
  Number of compounds owned by the user, which have already been moved to the common section of the customer database (for book-keeping).

- **SEQNOS_BELOW**
  Number of compounds in the common section not owned by the current user and having Customer RegNos below the user’s range (for book-keeping).

- **USER_DATA, USER_INDEX**
  Private files of a user. They contain compounds recently entered or replaced, but not yet moved to the common section. Names should be:

  - < CROSSFIRE root > /usr/<user name>/<database name>.udb
  - < CROSSFIRE root > /usr/<user name>/<database name>.uix

- **USER_INTNAME**
  Internal database name. Required to be identical to <user name> (in upper case).

- **USERSET**
  Directory of all compounds owned by a user independent of their storage in the private or common section, name:

  - < CROSSFIRE root > /usr/<user name>/<database name>.set
3.6 CrossFire Accounting System

The CrossFire Accounting System (XFAS) monitors all CrossFire related user activities on a server and stores the information into an ASCII file. The system administrator can use this file to calculate statistics and to do accounting.

The CrossFire Accounting System and its commands will only be available if an appropriate license is installed. Please use the command “show license” to check that the product “xfaccounting” is installed. If you do not see this product in the list of installed products then all commands described in this chapter will return the error message “DENIED”.

The architecture of the system guarantees that there is not much influence on the performance of the CrossFire system itself, because the accounting procedure is not a function of the MDL CrossFire Server but of the CrossFire daemon. It can be managed with XFMANAG.

The XFAS has the following basic features:

- Every (or a selection of) CrossFire related command(s) that has (have) been send from a user to the MDL CrossFire Server will be notified
- Accounting can be applied to one specific license group or to all groups of a server installation.
- The following information can be stored: User name, Group name, TCP Address, Database name, Database context, Process number, date, time, command name, elapsed time and CPU time
- The following commands of XFMANAG are used to control the accounting system:

  SHOW COMMANDS  Show commands being accounted.
                  If a name ends with an underscore, omit arguments.
  STOP ACCOUNTING  [/GROUP=group] : Stop accounting XFIRE commands.
  GET LOG       (<last> | <all>) : Display the log file contents. Show the last 20 (default) or (at most) 10000 lines.
  NEW LOG           Rename the current log file (new name is shown)
                    Rewrite the current file from its start.
  SHOW LOGNAME   Display the current log file name.
  INCLUDE COMMAND  {<command>} : Include commands into the log.
  EXCLUDE COMMAND  {<command>} : Exclude commands from the log.
START / STOP ACCOUNTING

Command Start / Stop Accounting

Entering „start accounting“ at the XFMANAG prompt will prepare the system for the accounting. In order to activate the accounting the command „refresh license“ has to be entered. „Stop accounting“ will close the accounting file. If you enter the optional parameter /GROUP=groupname, then the accounting will be started or stopped for this particular group.

3.6.1 LOGFILE HANDLING

Commands SHOW LOGNAME and NEW LOG

The accounting system is collecting the accounting information and writes it into a file which has the following default name:

<CrossFire system directory>/xfacct.log

Examples:

<table>
<thead>
<tr>
<th>AIX</th>
<th>/xfire/sys/xfacct.log</th>
</tr>
</thead>
<tbody>
<tr>
<td>WindowsNT</td>
<td>d:\xfire\sys\xfacct.log</td>
</tr>
</tbody>
</table>

The currently used name can be displayed using the command SHOW LOGNAME. New accounting information can be stored into another file using the command NEW LOG. This command will rename the old logfile XFACCT.LOG to a file with a number as extension, e.g. XFACCT.001. It will set the extension number automatically and will never delete an accounting file. New accounting information then is stored in a new file XFACCT.LOG.
**Command GET LOG** [ `<last>` / `<all>` ]

This command will display either the last 20 (default setting) or all entries of a log file. An entry has the following meaning (rows are separated using the pipe symbol `|`):

<table>
<thead>
<tr>
<th>ROW</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Time stamp with the format: YYYYMMDD:HHMMSS</td>
</tr>
<tr>
<td>2</td>
<td>User name + Group name (comma separated)</td>
</tr>
<tr>
<td>3</td>
<td>TCP/IP address + Client type and version</td>
</tr>
<tr>
<td>4</td>
<td>Process number</td>
</tr>
<tr>
<td>5</td>
<td>CPU time of the command</td>
</tr>
<tr>
<td>6</td>
<td>Elapsed time of the command</td>
</tr>
<tr>
<td>7</td>
<td>CrossFire database for which the command has been used. As an alternative the name HOME is used.</td>
</tr>
<tr>
<td>8</td>
<td>Database context of the command:</td>
</tr>
<tr>
<td></td>
<td>S Substance</td>
</tr>
<tr>
<td></td>
<td>R Reactions</td>
</tr>
<tr>
<td></td>
<td>C Citations</td>
</tr>
<tr>
<td></td>
<td>N no context found</td>
</tr>
<tr>
<td>9</td>
<td>Reference character for the kind of the command:</td>
</tr>
<tr>
<td></td>
<td>S structure search (for substances or reactions)</td>
</tr>
<tr>
<td></td>
<td>F or space fact search or another, not searching command</td>
</tr>
<tr>
<td>10</td>
<td>command word (see INCLUDE COMMAND) or the complete command</td>
</tr>
</tbody>
</table>

Example (one line):

```
@XFMANAGE> get log
20040224:113205|xfireadm,<group>|5814|0.00|0.00|HOME|N|INIT|0
20040224:113205|xfireadm,<group>|5814|0.00|0.00|HOME| |inhelp|0
20040224:113209|xfireadm,<group>|5814|0.00|0.00|HOME|N|EXIT|0
```
3.6.2 ACCOUNTED INFORMATION

Commands SHOW COMMANDS, INCLUDE COMMANDS and EXCLUDE COMMANDS

The accounting server is able to collect either specific commands or (if the command list is empty) all commands that a CrossFire user is sending to a MDL CrossFire Server. The command SHOW COMMAND will display the list of all monitored commands. The commands INCLUDE and EXCLUDE COMMAND will enhance or reduce the list of monitored commands.

A command word is the complete name of a MDL CrossFire Server command. If an underscore is added to a command word then only the name of the command but not the complete command will be stored.

The following commands are of importance for accounting:

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INIT</td>
<td>Start of a CrossFire session</td>
</tr>
<tr>
<td>EXIT</td>
<td>End of a CrossFire session</td>
</tr>
<tr>
<td>DBSELECT</td>
<td>Database selection</td>
</tr>
<tr>
<td>SEND</td>
<td>Display of hits</td>
</tr>
<tr>
<td>SEARCH</td>
<td>Search command</td>
</tr>
</tbody>
</table>

The following commands can also be included (please refer to section “Commands of the MDL CrossFire Server” for more detailed information on those commands):

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADDCOMP</td>
<td>Adds a new entry to the customer database currently selected</td>
</tr>
<tr>
<td>DBINFO</td>
<td>Returns textual information about the current database</td>
</tr>
<tr>
<td>DBLIST</td>
<td>Returns a data stream with keyword parameters about all databases available and their attributes</td>
</tr>
<tr>
<td>DELCOMP</td>
<td>Removes an entry in the current customer database</td>
</tr>
<tr>
<td>DELETE</td>
<td>Deletes a temporary or permanent hitset</td>
</tr>
<tr>
<td>Command</td>
<td>Description</td>
</tr>
<tr>
<td>-----------</td>
<td>--------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>DIR</td>
<td>lists either all hitsets from the current database or any hitsets available</td>
</tr>
<tr>
<td>DOWNLOAD</td>
<td>retrieves the ID numbers (i.e. BRNs, Customer RNs, reaction IDs, or citation IDs) from a range of hits in a hitset</td>
</tr>
<tr>
<td>EXPAND</td>
<td>renders a section of the index on a searchable database field</td>
</tr>
<tr>
<td>FINDGAP</td>
<td>returns the lowest RegNo in the current Customer database which is unused and may be written to by the current user</td>
</tr>
<tr>
<td>GETCFDIR</td>
<td>returns a range of lines from a datastructure table file (DST) stored at the server</td>
</tr>
<tr>
<td>REPCOMP</td>
<td>works identically to the ADDCOMP command with one exception; an existing entry under the RegNo specified is replaced</td>
</tr>
<tr>
<td>REPORT</td>
<td>renders the same information as is issued by the DBSELECT command for a Beilstein database</td>
</tr>
<tr>
<td>SM</td>
<td>this command is supported for backward compatibility only. It prompts back by <code>@SM&gt;</code> for the entry of a Rosdal string query.</td>
</tr>
<tr>
<td>STORE</td>
<td>copies an existing hitset to a new hitset</td>
</tr>
<tr>
<td>UNLOAD</td>
<td>Retrieves the query which gave rise to a hitset</td>
</tr>
</tbody>
</table>

A change of the list of the monitored commands is only taken into account for those CrossFire sessions that run after the change has been made.
3.6.3 XFIRE.INI AND XFIRED.CFG

The following lines in the XFIRE.INI file (located in the bin directory of the MDL CrossFire Server installation) define the accounting system settings:

Example:

```
[INSTALLATION]
ACCOUNTHOST=LOCALHOST;
ACCOUNTPORT=8002;
ACCOUNTING=ON;
```

The following lines in the XFIRED.CFG file (located in the sys directory of the MDL CrossFire Server installation) define details for the accounting:

Example:

```
[Accounting]
Port=8002;
AccountCommands=search_,,send_,,dbselect,init,exit;
AccountLog=/xfire/sys/xfacct.log;
```
3.7 The CrossFire System in Multi-Server Environments

It is possible to couple multiple instances of Xfire daemons on different machines in order to increase performance and to ensure that licenses are managed from one of the instances only, the master instance. The other (slave) instances first try to access the master for getting a product license and make use of its own licenses (if any) only in case of a failure.

a. Each of the instances has to be installed as a normal Xfire server. The slave instances must reside on the same platform, the master instance may be on a different platform.

b. Each slave must be able to run with the same xfire.ini file. This file has to be identical in all BIN directories including the master. This means that all slave machines must have the same file system layout.

c. The master may or may not respond to local xfire server processes. If it does, it must also have the common file system structure. Otherwise, at least all names of DST files in xfire.ini must be valid.

d. Each slave needs an additional entry in xfired.cfg:

    ...
    [Licensing]
    ...
    Master=<dotted IP address>;


e. In the master xfired.cfg, all slaves must be listed:

    ...
    [Licensing]
    ...
    Slaves=<list of dotted IP addresses (commas)>;
3.8 CrossFire Licensing

3.8.1 INSTALL A LICENSE

Licenses are created and delivered by Elsevier MDL. They are ASCII strings stored in files with the extension “*.xfl” and can be delivered on diskette or via e-mail.

Licenses are installed using the program XFMANAG. Ensure that you have copied your license file into the sys directory of the MDL CrossFire Server and that it is readable (i.e. it is recommended to open the license file using a normal ASCII editor to check for any special characters. If characters such like "^M" etc. are visible then this has to be corrected.)

Switch to the CrossFire sys directory and run XFMANAG:

```
d:\xfire\sys>xfmanag
(Note: if port numbers other than the default settings have been used then XFMANAG has to be called with the following parameters: „xfmanag localhost <port No>“. XFMANAG expects to establish a connection to the CrossFire system using the licensing port, which is defined in the file XFIRED.CFG. Default: 8004)

[control client prompt]
@XFMANAGE>set lic /localfile=nt.xfl
```

Several messages will be shown on the screen. If no error occurs then you will get the hint to use the command “refresh license” to activate the installed license.

```
[. . . system messages]
@XFMANAGE>refresh lic
```

This command will send a command to the CrossFire service and will activate the license. If you have got an error message in the step before then please check the license file and contact Elsevier MDL.

The following commands will create a complete XFIRED.CFG file, which is used by the CrossFire daemon. If you will get the message “DENIED” then you can ignore it at this stage.

```
@XFMANAGE>set dump on
@XFMANAGE>set dump off
```

Now the new license is installed and you can exit XFMANAG using the command “quit”.

```
@XFMANAGE>quit
```
3.8.2 LICENSING COMMANDS

3.8.2.1 Read a license file

As described above license files are ASCII files, which contain the necessary License information. The following command reads this license information:

```
SET LICENSE [/LOCALFILE=<filename>] [/KEY=<encoded>]
[/PRODUCT=...] [/UID=...] [/STATION=...][/NAME=...]
[/GROUP=...] [/COUNT=...]: Add or update license.
```

The functions of this command are:

- **Getting product licenses from a license file**

  `/LOCALFILE=<filename>`

  The license file should be transferred to the `\fire\sys` directory prior to installation. One License file may contain licenses for one or more CrossFire group.

  Manual entering of a single product license

  `/KEY=<encoded>`

  (The encrypted text has to be entered manually.)

- **Adding a named user**

  `/GROUP=... /PRODUCT=... /UID=... [COUNT=...]`

  (The default setting for GROUP is „DEFAULT“. A user can be entered several times and can log into the system several times.)

- **Adding a registered station using a station ID and a station name (option).** This function should only be used if anything needs to be fixed. The CrossFire client will use it automatically.

  `/GROUP=... /PRODUCT=... /STATION=... [NAME=...]`
3.8.2.2 Clear License

CLEAR LICENSE [/PRODUCT=...] [/UID=...] [/STATION=...]
[/GROUP=...] [/COUNT=...]: Modify license.

This command can only be used if the appropriate license has been installed. The system administrator can use this command to manage named accounts and seat licenses. Related topic: Command Set License

- Remove a whole license group
  
  [/GROUP=...]

- Remove a named user
  
  [/GROUP=...] /PRODUCT=... /UID=... [/COUNT=...]

  (a user, which has been entered several times can be removed several times)

- Remove a registered station with the station ID:
  
  [/GROUP=...] /PRODUCT=... /STATION=...

3.8.2.3 Refresh new license information

REFRESH LICENSE Make new license state available to users.
TRY LICENSE Try loading the current license state for check.

Every change of a license and every manual change of XFIRED.CFG and XFIRE.INI will only be entered into the .LIC files first. The command TRY LICENSE allows to check, whether any modification will cause an error or not. If TRY LICENSE will return with no error, then the command REFRESH LICENSE will activate the changes for the system.

Currently active users will be deactivated and reactivated with the new license information. This may fail if the new license will be a limitation to a previous license.

3.8.2.4 Display the licenses

SHOW LICENSE [/PRODUCT=...] [/GROUP=...]: Display license.

This display command works in the same way like the GROUP command.
3.9 CrossFire Messaging

The MDL CrossFire Server is able to send messages to users of the system on request of a MDL CrossFire Commander client. The MDL CrossFire Commander will ask the server for messages on logon and after that it sends a request for messages every two minutes (polling mechanism). If there is a new message available then it will be displayed in a dialog box. All available messages will be collected and displayed together in one dialog box. If the message contains URLs then these will be filtered and displayed in a new dialog box, where they are presented as hyperlinks.

When you specify a URL e.g. http://www.mdl.com/crossfire in the message text the Commander will directly link users to this page. If you want to make the linking optional you have to add HOMEPAGE= to the URL, and write HTTP in capital letters, e. g. HOMEPAGE=HTTP://www.mdl.com/crossfire

Messages are plain ASCII text files, which can be located in the CrossFire <usr> directory. If a different directory should be used then the path to this directory has to be entered in the file XFIRE.INI under section [CONFIG] after the keyword MESSAGEPATH=.

If messages should be sent to specific user groups (only available for installations with a multi user group licensing), the text files can be put into the <usr> directory of the group. The MDL CrossFire Server will collect all messages located in the <usr> directory and in the directory specified by the keyword of the XFIRE.INI file.

Note: changes of the XFIRE.INI file will only become active if the command "ref lic" is used in the program XFMANAG.

The system distinguishes between four types of messages:

- Logon messages (file name: logon.xms)
- Info messages (file name: info.xms)
- Urgent messages (file name: urgent.xms)
- User specific messages (file name: <user id>.xms)
3.9.1 LOGON MESSAGES
The contents of the file "logon.xms" will be sent to every user once on every logon.

The file can be located either in the <usr> directory of the CrossFire installation or in the directory specified in the message path keyword of the XFIRE.INI file.

If the message should not be sent any longer than this file has to be renamed or deleted.

3.9.2 INFO MESSAGES
The contents of the file "info.xms" will be sent to every user, who is already logged into the system and to every user, who starts using the system.

The file can be located either in the <usr> directory of the CrossFire installation or in the directory specified in the message path keyword of the XFIRE.INI file.

If the message should not be sent any longer than this file has to be renamed or deleted.

3.9.3 URGENT MESSAGES
The contents of the file "urgent.xms" will be sent only once to every user, who is logged into the system. New users will not get this message. If the administrator does not want to send the message to every user but only to specific users, then the administrator can create a user filter. The file "urgent.flt" should contain a list of those user names, which should get the message. If this file is missing then the message will be sent to every user of the system. If the contents of the files "urgent.xms" and "urgent.flt" will change then the message will be send again.

The server will create a file "urgent.log", which will contain a read confirmation for every user, who has got the message (time stamp). This file should be deleted, if the purpose of the message has been fulfilled. A user should get the message at latest 10 minutes after it has been created.

The file can be located either in the <usr> directory of the CrossFire installation or in the directory specified in the message path keyword of the XFIRE.INI file.

If the message should not be sent any longer than this file has to be renamed or deleted.
3.9.4 USER MESSAGES

The contents of the file ",user name">.xms" will be sent to the user with the same name once a session. The user will get the message again, if he tries to open a new session.

The file can be located either in the <usr> directory of the CrossFire installation or in the directory specified in the message path keyword of the XFIRE.INI file.

If the message should not be sent any longer than this file has to be renamed or deleted.

Example Message:

Use any text editor to write the following text (without quotes):

“"This is a test message for all users. You will find additional information on MDL products if you checkout the following web page:

http://www.mdl.com

If you have any further question, please contact your local administrator.”

Then save this text with the name “logon.xms”. Copy this file into the USR directory of the MDL CrossFire Server using FTP and ensure that it transferred using ASCII mode. Once the file is available in the usr directory every CrossFire user will see this message in a dialog box and he will be able to open the http hyperlink.
3.10 MDL CrossFire Server Appendix

3.10.1 TECHNICAL REQUIREMENTS AND INFORMATION

3.10.1.1 Supported Platforms

<table>
<thead>
<tr>
<th>Supported Platforms</th>
<th>Intel based PCs, IBM RS6000, SUN SPARC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating System</td>
<td>AIX 4.3x - 5.2 , MS Windows NT , Windows 2000, Windows 2003</td>
</tr>
<tr>
<td>Memory (minimum)</td>
<td>64 MB Ram (AIX) / 128 MB (NT)</td>
</tr>
<tr>
<td>Tape Drive</td>
<td>DLT Tape IV compatible such as Quantum Compac DLT 4000</td>
</tr>
</tbody>
</table>

3.10.1.2 Diskspace

SERVER FILESYSTEM STORAGE

The server requires only about 50 MB, but additional disc space is needed to save hitsets during a session. You also need disk space to store intermediate hitsets. As a minimum we recommend 100 MB per User. You can assign / distribute the disk space according to your needs with xfmanag, please refer to 3.3.7 The CrossFire Manager Control Program “xfmanag”.

DATABASE STORAGE

| CrossFire Beilstein | 52 GB Storage Space* , ** |
| CrossFire Gmelin    | 11 GB Storage Space** |

* The database will grow with approx. 2 Gbyte per year. Please refer to the filelist paper for more details on the necessary disk space.

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Note: If the customer wants an uninterrupted database service while installing a new database version he needs to double the disk space. Otherwise the service has to be interrupted for 8-10 hours (depending on the tape drive) when installing a new database version of CrossFire Beilstein.
3.10.1.3 The CrossFire Communication Protocol

With this protocol CrossFire is using a proprietary encryption mechanism which works as follows:

A symmetric key V is used in a way that a message (data packet) m encrypted with V will be decrypted using V again: V(V(m))=m.

The key is not sent over the network but only a so called "seed" value, this value has a length of 128 bit. The seed value is a random string created by that side which tries to initiate the encryption protocol (in case of CrossFire the client, the Beilstein Commander) using the MD5 algorithm. Either on the client side as well as on the server side algorithms are implemented which can create the actual key out of a seed value.

The key will be modified every time a message is sent, which means that every message exchange will use a different key. Client and server will do the modification synchronously. TCP is a secure protocol which means that no interference/disturbance should happen. However, if this will happen in any case then this will be recognized and the encryption will be re-initialized. Before an encryption will start, messages will be compressed. The reason why compression starts first before the encryption is that ASCII text can be better compressed than binary files. The compression algorithm works with a fixed Huffman code.

The encryption of the xfire protocol will be enabled by a special license string XfEncryption which is part of the license file. If this string is not present, only UserID and Password will be sent encrypted. The encryption is valid for the whole crossfire group.
1. establishing a connection through the client (default port: 8001)

2. CrossFire daemon “xfired” (or xfire service in case of Win NT / 2000) launches one dispatcher per client (default port: 8002). Dispatcher inherits connection to client from xfire (default port: 8001).

3. Authentication and Encryption (if enabled)

4. Start of the MDL CrossFire Server “xfire”, communication via sockets

5. xfire checks xfire.ini, licensing and accounting (default port 8002 is used for licensing, default port 8003 for accounting)

6. XFMANAG is used for controlling the daemon (licensing and accounting) (default port: 8004)
3.10.1.5 Directory Structure

<XCrossFire Root Directory> (usually called xfire)

ALERT (contains the alert profiles of several users)

BIN (contains the MDL CrossFire Server software and the XFIRE.INI file and also the automatically created database images)

SYS (contains the maintenance tools, the CrossFire control client XFMANAG and the CrossFire daemon)

TMP (is used for storing temporary files)

UPDATE (is the working directory for incremental updates)

USR (is used by the MDL CrossFire Server for creating and storing user hitsets)

DB (contains several other directories or only one, which will be used for storing the database files. Needs not to be under the CrossFire root directory, but needs to be a recognizable file system, e.g. the name of the file system must not contain capital letters under AIX. Please refer to the chapter about XFMAINT for the limitations of this program.)
### System limits of the Server

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>User database, disk space</td>
<td>approx. 1,5 KB per structure</td>
</tr>
<tr>
<td></td>
<td>approx. 6 KB per reaction</td>
</tr>
<tr>
<td>Workspace for storing temporary hitsets</td>
<td>10-20 MB per concurrent user</td>
</tr>
<tr>
<td>Maximum number of databases</td>
<td>40</td>
</tr>
<tr>
<td>Maximum compounds per customer database</td>
<td>64,000,000</td>
</tr>
<tr>
<td>Maximum number of users</td>
<td>unlimited</td>
</tr>
<tr>
<td>Virtual memory per user recommended</td>
<td>32 MB</td>
</tr>
<tr>
<td>Maximum size of one query</td>
<td>24 K</td>
</tr>
<tr>
<td>Maximum number of heavy atoms per structure</td>
<td>1600</td>
</tr>
<tr>
<td>Maximum number of bonds</td>
<td>4800</td>
</tr>
<tr>
<td>Maximum number of fragments</td>
<td>128</td>
</tr>
<tr>
<td>Maximum number of markush groups and atomlists</td>
<td>64</td>
</tr>
<tr>
<td>Maximum of bond change requests per reaction</td>
<td>50</td>
</tr>
<tr>
<td>Inactivity timeout</td>
<td>Variable</td>
</tr>
<tr>
<td>Activity timeout</td>
<td>24h</td>
</tr>
</tbody>
</table>
3.10.2 BEILSTEIN / GMELIN DATABASE FILE DATA ORGANIZATION

The following section is a brief survey of the Beilstein database organization.

The Beilstein database is a collection of data units or records. Three different types of data units are distinguished:

- Substances or Compounds
- Reactions
- Citations

The data unit types will usually be termed contexts. An ID number uniquely identifies each item of a data unit with one of the three types:

<table>
<thead>
<tr>
<th>Context</th>
<th>ID Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances</td>
<td>Beilstein / Gmelin Registry Number (BRN /GRN)</td>
</tr>
<tr>
<td>Reactions</td>
<td>Reaction ID Number (RX.ID)</td>
</tr>
<tr>
<td>Citations</td>
<td>Document ID Number (CNR)</td>
</tr>
</tbody>
</table>

A data unit is subdivided into sections termed properties; each property is further subdivided into fields. Properties and fields are identified by names.

In all three contexts, two types of properties are distinguished:

Each data unit has exactly one ID property containing its ID number as a data field.

A data unit may possess one or more additional non-ID properties each being identified by a name. The same property may occur repeatedly.
The three contexts are interrelated in the following manner:

<table>
<thead>
<tr>
<th>Pair of Contexts</th>
<th>Relation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances and Citations</td>
<td>Any property of a substance may include a (multiple) field containing citation ID numbers identifying the original document the information was taken from. This does not apply to ID properties.</td>
</tr>
<tr>
<td>Substances and Reactions</td>
<td>The reaction ID property includes two fields listing the reactants and products of the reaction. Those fields contain BRNs.</td>
</tr>
<tr>
<td>Reactions and Citations</td>
<td>The (only) reaction non-ID property refers to citations like in the case of substance non-ID properties.</td>
</tr>
</tbody>
</table>

By the relations described, any (source) item in a particular context gives rise to a list of (target) items in a different context in one of two ways:

The target item ID numbers are the set of all ID numbers contained in the source item data.

The target items are all those items in the target context containing the source item ID number in one of their data fields.

The context relationship is encountered when performing certain CROSSFIRE commands:

A set of source context items (e.g. a hitset resulting from a query) may be converted to a different target context by applying the above context switch to any member and uniting all target items to a set. This is an option to a CROSSFIRE SEARCH command.

A non-ID property in the substance or reaction context includes an abbreviated representation of all citations referenced from it.

In the display of a substance, all reactions are included referring to the current substance either as a reactant or a product. What is shown is the ID property of a reaction, one occurrence of the non-ID properties, and the citations attached to it.

Displaying a citation also yields the substances and reactions referring to the current citation in at least one of their properties. Reactions are displayed as described above.
3.10.3 CUSTOMER DATABASES

3.10.3.1 Creation and Maintenance

3.10.3.1.1 Introduction

In addition to using the Beilstein or Gmelin database, which are “read-only” databases, you can load structures of your own into one or more customer databases. Such customer databases offer the following features:

Every structure intended for storage in a customer database must be provided with an identification number in the range 1 to 67882064 (= $2^{26}$). Presently, there is no control mechanism implemented to ensure that different ID numbers must represent chemically different structures.

The source of structures loaded into a customer database may be an input file in a special format described later. The CROSSFIRE maintenance software offers a “load” option to enter such files into a customer database in one or several repeated batches.

If users are assigned to a customer database, they have the capability to individually enter proprietary structures using the structure editor of the CROSSFIRE Client software.

Note that a user is not automatically enabled for this task by means of membership of the xfire group, but must be made explicitly known to the MDL CrossFire Server. At that time, a range for the ID numbers of the particular user must be defined. Other xfire users without this authorization still have read access to any customer database.

Immediately after input, only their owner keeps user structures in private files where they are visible and searchable. By means of a “collect and load” process, the administrator is able to move user structures into a common section of the customer database where they are visible and searchable by all users, but still modifiable only by their owner. Any modifications are at once visible to the owner, but to other users only after the next “collect” operation.

A customer database may be designed to receive only batch, or user input, or both. In the last case, structures entered in batch should be assigned ID numbers from the lower end of the ID number range, say 1 to 32,000,000 with a lowest user ID number of 32,000,001.

A user logged in under the CROSSFIRE administrator’s ID should do all tasks described in this chapter.
3.10.3.1.2 Creation, Back-up, and Removal of a Customer Database

In addition to the delivered CrossFire you may define customer databases:

a) Start the CROSSFIRE maintenance program from the directory 
   
   `<CROSSFIRE root>/sys` (usually `/xfire/sys`):
   
   ```
   cd `<CROSSFIRE root>/sys
   xfmaint [<CROSSFIRE root>]
   default: /xfire
   ```

b) Be sure (e.g. by using option 1 to view the CROSSFIRE file systems) that sufficient space is available for the new database. Due to empty data blocks the initial size is about 320 Kbytes.

c) Select option 3 from the main menu, then select option 2. You are prompted for the name of the customer database to be created. Enter a name of, at most, 19 characters and consisting of letters, digits, and underscore characters. Database names are not case sensitive. To prevent later problems, choose a name that is unique within the entire system.

d) After a positive reply to a confirmation, an empty customer database is created which is initially in a disabled state. If you intend to load batch structures leave the database disabled. Otherwise, if you want to define users authorized to update, enable the database with menu option 4.

A customer database (as well as a Beilstein / Gmelin database version) may be backed-up to tape using the following instructions:

a) Start the CROSSFIRE maintenance program from the directory 
   
   `<CROSSFIRE root>/sys` (usually `/xfire/sys`):
   
   ```
   cd `<CROSSFIRE root>/sys
   xfmaint [<CROSSFIRE root>]
   default: /xfire
   ```

b) Select option 2 from the main menu to get a list of all databases currently installed. Select a database by its number # entering “b#”.

c) You are prompted for the following information:

   the approximate capacity of a tape cartridge in bytes. If the blocksize of your tape drive has been set to 2048 bytes, a value of 1,940,000,000 bytes (enter it without the commas) is appropriate. The value established will be retained for later use.

   The program will answer with the number of tape cartridges required for all database files.

   In the following dialog you will be asked for:
the tape label (for your convenience)
the name of the output tape device. Names are “/dev/rmt#”, the default is “/dev/rmt0”

To execute the script, leave the maintenance program. You will be prompted for
insertion of the first and subsequent tape cartridges. The time for writing a completely
full cartridge is about 2.5 hours.

A customer database or Beilstein file version may be removed as follows:

a) In case of a customer database, all users enabled for updates of that
database have to be removed first, following the instructions in the next
section.

b) Start the CROSSFIRE maintenance program from directory “<CROSSFIRE
   root>/sys” (usually “/xfire/sys”):

   \texttt{cd <CROSSFIRE root>/sys}
   \texttt{xfmaint [<CROSSFIRE root>]}\hspace{2cm} \text{default: /xfire}

   \texttt{c) Select option 4 to disable the database before it can be removed. Select the
database to be disabled using “d#” where # is its number in the database
table shown.}

   Disabling will fail if there are active CROSSFIRE users on the system (even if
they have selected different databases).

   d) To execute the database removal, select option 2 from the main menu and
   specify the database using “r#”. After a confirmation, the maintenance
   program will delete all references to the database from the CROSSFIRE
   configuration file. To delete the database files also, it writes a shell script

   \texttt{<CROSSFIRE root>/sys/del.bat}

   Usually /xfire/sys/del.bat. This script can either be executed from xfmaint or
after leaving the maintenance program.
3.10.3.1.3  Administration of Users Authorized for Updates

A customer database may have users authorized to store proprietary structures that were entered under the structure editor of the CROSSFIRE Client. Other users in the “xfire” group may have only read access to a customer database.

To enable xfire users to have update access to a specific customer database, take the following steps:

a) Start the CROSSFIRE maintenance program from directory “<CROSSFIRE root>/sys” (usually “/xfire/sys”):

   ```
   cd <CROSSFIRE root>/sys
   xfmaint [<CROSSFIRE root>]
   default: /xfire
   ```

b) Be sure that the database to be affected is currently enabled using option 7 of the main menu.

c) Select option 2 of the customer database menu to get a list of all customer databases currently defined. Select the desired database by its number.

d) You are prompted for selection ‘l’ (list users), ‘a’ (add a user), ‘r’ (remove a user), or ‘e’ (exit to the main menu). Select ‘a’, possibly after viewing the list of all previously defined users with ‘l’.

e) You are prompted for the name of the user to be added. This user must be a member of the xfire group. Acceptable user names may contain letters, digits, and underscores and a maximum of 19 characters. Uppercase and lowercase letters are not distinguished.

f) Next, you are prompted for the lowest customer RegNo the future user may assign to proprietary compounds. For the first user, any number in the range 1 to 67,108,864 (omit the commas) may be specified. However, consider the planned database layout as described at the beginning of this chapter. For any subsequent user, the program suggests the lowest possible number as the lower limit. You may decide to enter a higher number.

g) Finally, you are prompted for the number of RegNos assigned to the future user. After that, the program will create several files for the storage of proprietary compounds and add the current user to the user table.

h) User file creation will fail if the new user’s RegNo range includes compounds already present in the customer database. In this case, the program prints the currently highest RegNo of the database. Choose a lower limit above that value in a second attempt to add the user.
Conversely, you may wish to remove users from the user table of a database:

a) Start the CROSSFIRE maintenance program from the directory “<CROSSFIRE root>/sys” (usually “/xfire/sys”):

   
   $ cd <CROSSFIRE root>/sys
   $ xfmaint [<CROSSFIRE root>]
   
   default: /xfire

b) Be sure that the database to be affected is currently disabled using option 4 of the main menu. Disabling will fail if there are active CROSSFIRE users on the system (even if they have selected different databases).

c) Select option 2 of the customer database menu to get a list of all customer databases currently defined. Select the desired database by its number.

d) Select ‘r’. You are prompted to enter the name of the user to be removed.

3.10.3.1.4 Loading Customer Structures in Batch Mode

Compounds with RegNos outside any user range may be loaded into a customer database in batch mode. At the time of a load operation, existing compounds may also be replaced or deleted.

As the input of a load operation you have to provide 3 files. All of them must exist (even if as zero length files) and be readable by the CROSSFIRE administrator:

The structures to be added, or to replace existing compounds, must be available in a special type of file called “Rosdal wrapped into SDF”. Such files are prepared as follows:

Provide a text file where each line represents a Beilstein Rosdal string according to the published format specifications. As an additional requirement, each Rosdal string must contain a unique Customer RegNo as value to the “CRN” keyword.

Use the program <CROSSFIRE root>/sys/xfwrap to generate the required load input file. Parameters are:

   $ xfwrap <in file> <out file> <mode>

The mode parameter is ‘W’ (default) for the required file conversion and ‘U’ for the inverse process, restoring a text file.

The maximum file size loadable in a single step is limited to 320,000 Kbytes. No compound affected by a batch update can be owned by a user enabled for customer database updates.

For any structure replacing a previously loaded one and for any compound to be deleted from a customer database, an entry to a “search deletion list” (text file) is
required, specifying the Customer RegNo to be affected. Each entry is a text line with a RegNo as a decimal numeric string.

The search deletion list will remove RegNos from the substructure search files of the customer database. The process only affects data in the previous generation of the search files, not those resulting from the current load file.

**Note:** If a load file contains a RegNo already present in the database and if there is no corresponding search deletion list entry, an inconsistent state of the database will result.

For any structure to be deleted an entry to a second deletion list ("data deletion list") is required. A data deletion list consists of RegNos (one per line) with the appended letter ‘D’. Entries will cause the removal of compounds from the display section of the customer database.

**Note:** Inconsistencies between the search and data deletion lists will cause incorrect database behavior.

After preparation of the load file and the search and data deletion lists, an update operation to a customer database can be done using xfmaint:

a) It is recommended that a database backup should be written before any sequence of major update operations. Follow the instructions in the chapter "Software and Database Installation".

b) Be sure that the database to be affected is currently disabled using option 4 of the main menu.

c) Select option 4 of the customer database menu. You are prompted for the 3 names of the load file and the search and data deletion lists. Enter the names of existing files in each case. The possibility of using default file names is restricted to the “collect and load” operation of chapter "Collecting and Loading ...".

Based on the input file sizes, the maintenance program checks in advance for sufficient space for the extension of database files and the allocation of additional database files and temporary work files. All required space is claimed from the file systems currently assigned to CROSSFIRE. To ensure successful processing, the total space required is overestimated considerably. If the program denies the load operation due to insufficient space, try one of the following measures:

- Add a new, or increase an existing, file system - refer to chapter "Software and Database Installation".

- Reduce the size of the load file, i.e. split it into a succession of smaller files.

It may happen that a file is required to grow within its file system when a free space is occupied by the files not affected by the update, e.g. files from another database. The
maintenance program issues a message for the particular file encountering that problem. The solution is to move files to other file systems and reattempt the operation. However, the new full file names must be inserted into the CROSSFIRE configuration file by manual editing. Refer to chapter "Details on File loading ..." for details. Before a new attempt to start the load operation, you should have the installation verified using menu option 8 (see chapter "Validating the CrossFire Installation").

d) If successful in achieving all the required space, the maintenance program writes a shell script

<crossfire root>/sys/load.bat

to be executed after exiting to the shell level. After successful script completion, re-enable the database.

3.10.3.1.5 Collecting and Loading Proprietary User Structures

For a customer database with write access users, a "collect and load" process may be executed for one of two reasons:

• Make user structures visible and searchable to users other than their owner.

• Increase the speed of substructure searches for users who have entered a large number of compounds.

The total process consists of a collect step and a load step that is analogous to the description in the chapter "Loading Customer Structures ...". The collect step provides for the 3 input files of the load step, the scanning of all user specific files. The subsequent load step performs the following actions:

All required updates are applied to the common section of the customer database.

In addition to batch load processing, all private user files are cleared (since all user compounds were moved to the common section).

First select menu option 5. This may be done at any state of a customer database and does not make any changes. You will see a listing of all user compounds (it will also be written into the file VERIFY.LOG, so that it can be reviewed later with any text editor).

After this, follow the instructions in the chapter "Loading Customer Structures ...", but enter an empty line when prompted for the name of the load file.
3.10.3.2 File loading Procedures

3.10.3.2.1 General

As indicated earlier, the common section of a customer database comprises 5 types of files:

SEARCH (file set), INDEX (single file), and TREE (set of 11 members) files are used for substructure search. The compounds originally entered are stored and retrieved for display using file types COMMON_DATA (file set) and COMMON_INDEX (single file).

Structures to be added to the search and display files, or intended to replace structures in a previous file generation, have to be provided in a special format described in chapter "Customer Databases ...". Conversion from "one Rosdal per line" format or (in future versions) further input formats is done by the program "xfwrap".

The display files are fully capable of random updates when receiving structures with identification numbers (also termed Customer RegNos) already present.

For the search files, a replacement must be accomplished by a deletion of RegNos being replaced from the old data generation plus an addition of different structures under the same RegNos. Furthermore, updates initially will only apply to the set of SEARCH files. After SEARCH update completion, the TREE and INDEX files have to be rewritten.

Both search and display files allow for deletions of RegNos specified in a text file list.

The following topics will be described:

• Initial loading of the search and display files.
• Merging several search file sets.
• Updates to search files and to display files (indexed update and mass update).

The file loading procedures described below are an alternative to the automatic database updates offered by the CROSSFIRE maintenance program. They should be considered especially for large databases where storage requirements and execution time may be a problem. However, they are inappropriate for customer databases with update-enabled users.
3.10.3.2.2 Initial Loading of the Search Files

All search files of a customer database may be generated in a single step using the following shell script:

```
#########################################################
# Generate search files of a customer DB in a single step
#########################################################
########################## paths/files/constants
PGM=/xfire/sys/          # program path
W=/xfire/tmp/            # temp path
P=/xfire/db/filesys/     # data path (target file system)
DBNAME=custdb            # database name
INPUT=sdf.dat            # input file name
BLOCKSIZE=16384          # SEARCH and TREE blocksize
I_BLOCKSIZE=32000        # INDEX blocksize
MAXBLOCKS=20000          # max. # of blocks per SEARCH component file
REPORT=10000            # report progress for coding and trees
########################## error exit
errquit() { echo "*** ERROR in program $*" ; exit 1 ; }
########################## code
cat <<END >${W}input
SDF=${P}$INPUT;
STRING=${P}string.dat;
CODE_BRN=YES;
CODE_FROM=1;
CODE_TO=1000000;
SCAN=NO;
DUMP=NO;
REPORT=$REPORT;
END
${PGM}xfcode ${W}input || errquit xfcode
########################## sort
cat <<END >${W}input
INFILE=${P}string.dat;
OUTFILE=${P}string.out;
PATH=${P};
NSTRING=100000;
NBUF=60;
IOSIZE=300000;
END
${PGM}xfsort ${W}input || errquit xfsort
rm ${P}string.dat
########################## compress
cat <<END >${W}input
STRING=${P}string.out;
OUTSEARCH=${P}$DBNAME.s1,
$P$DBNAME.s2,
$P$DBNAME.s3;
BLOCKSIZE=${BLOCKSIZE};
MAXBLOCKS=${MAXBLOCKS};
```
VERSION=100;
END
${PGM}xfcomp ${W}input || errquit xfcomp
rm ${P}string.out

########################## build search index

```bash
cat <<END >${W}input
    SEARCH=${P}$DBNAME.s1,
    ${P}$DBNAME.s2,
    ${P}$DBNAME.s3;
    INDEX=${P}$DBNAME.idx;
    BLOCKSIZE=${I_BLOCKSIZE};
END
${PGM}xfindex ${W}input || errquit xfindex
```

END

```
########################## build tree files

```bash
cat <<END >${W}input
    SEARCH=${P}$DBNAME.s1,
    ${P}$DBNAME.s2,
    ${P}$DBNAME.s3;
    TREE=${P}$DBNAME.t0,$P$DBNAME.t1,
    ${P}$DBNAME.t2,$P$DBNAME.t3,
    ${P}$DBNAME.t6,$P$DBNAME.t7,
    ${P}$DBNAME.t8,$P$DBNAME.t9,
    ${P}$DBNAME.t10;
    TREESIZE=10;
    BLOCKSIZE=${{BLOCKSIZE}};
    REPORT=${REPORT};
END
${PGM}xftree ${W}input || errquit xftree
```

Description:
The input structures are coded to a file of searchable records called bitstrings. This
file is sorted and then compressed to a SEARCH file (set). Non-first components of
that set are created only if the MAXBLOCKS limit is surpassed. It is useful to specify
an overestimated number of components.

Based on the SEARCH file set, an INDEX file and 11 TREE files are created for
substructure search purposes. The single file system referenced in the above script is
no requirement. In fact, each file (especially components of a set) might have it's own
path name.

The BLOCKSIZE and MAXBLOCKS values should be the same on the entire
system.

Space:
An upper limit of the final space required is twice the size of the input file. The
intermediate space requirement is three times that size.

Time:
Coding, sorting, and compression will take 0.1 sec per compound (order of
magnitude only), tree file creation 0.01 sec. Index creation time is negligible.
### 3.10.3.2.3 Merging Search File Sets

Large databases (more than 200,000 compounds) should not be built in one step. Instead, the processing as described in the previous section should stop after compression to yield a SEARCH file from a reasonably large input portion. The resulting SEARCH portions can be merged using scripts like:

```
# Merge multiple SEARCH sets to one SEARCH set
PGM=/xfire/sys/              # program path
W=/xfire/tmp/                # temp path
P=/xfire/db/filesys/         # data path (target file system)
SET1=custdb1                 # input set 1: 2 component files
SET2=custdb2                 # input set 2: 2 component files
SET3=custdb3                 # input set 3: 1 component file
DBNAME=custdb    # output SEARCH file
MAXBLOCKS=20000           # max. # of blocks per component file

# component file
errquit() { echo "*** ERROR in program $*" ; exit 1 ; }

# component file
cat <<END >${W}input
INFILES=
&P$SET1.s1,$P$SET1.s2+
&P$SET2.s1,$P$SET2.s2+
&P$SET3.s1;
OUTSEARCH=$P$DBNAME.s1,
&P$DBNAME.s2;
MAXBLOCKS=$MAXBLOCKS;
END
${PGM}xfmerge ${W}input || errquit xfmerge
```

One or more input SEARCH files or sets may be specified on the INFILES keyword using plus signs as separators. Components within a set are, as before, separated by commas.

For the resulting SEARCH file (set), INDEX and TREE generation would have to proceed as for an initial loading only applying the above steps “build search index” and “build tree files”.
### Updating Search Files

An existing SEARCH file (set) may be extended by the contents of a SEARCH file (set) to be added, while at the same time compounds may be deleted from the updated file (set):

```plaintext
# Update a search file set

PGM=/xfire/sys/          # program path
W=/xfire/tmp/            # temp path
P=/xfire/db/filesys/     # data path (target file system)
DBNAME=custdb            # database name
ADD=search.new           # SEARCH file to be added
DELLIST=delete.lst      # deletion list name (line: <RegNo>)
MAXDEL=100               # delete 100 compounds
               # database DBNAME requires its presence
               # in files ADD and DEL
MAXBLOCKS=20000          # max. # of blocks per SEARCH component file

errquit() { echo "*** ERROR in program $*" ; exit 1 ; }

The above script assumes an old SEARCH file of 2 components (keyword UPDSEARCH) and a maximum of 2 further components (keyword OUTSEARCH) to be created on overflow at the MAXBLOCKS limit.

The final space for old, and possible new, SEARCH components is required to grow by, at most, the size of the ADDSEARCH file. Furthermore, work space (file SWAPNAME) is required with 110% size of the ADDSEARCH file.

On completion, new INDEX and TREE files have to be rebuilt as described for the merge process. A failure of the update run is destructive to the update SEARCH file set.
```
3.10.3.2.5 Initial Loading of Display Files

The following script loads customer structures (SDF file with enwrapped Rosdal strings) into one or more components of a data file and then builds an index file:

```bash
# Generate display files of a customer DB in a single step
# paths/files/constants
PGM=/xfire/sys/ # program path
W=/xfire/tmp/  # temp path
P=/xfire/db/filesys/ # data path (target file system)
DBNAME=custdb  # database name
INPUT=sdf.dat  # input file name
BLOCKSIZE=16384 # display file blocksize
MAXBLOCKS=20000 # max. # of data file components

# error exit
errquit() { echo "*** ERROR in program $*"; exit 1; }

# load data file
cat <<END >${W}input
SDF=$P$INPUT;
DATA=$P$DBNAME.d1,$P$DBNAME.d2;
INTNAME=CUSTOMER;
TEMP=${P}temp.tix;
BLOCKSIZE=$BLOCKSIZE;
MAXBLOCKS=$MAXBLOCKS;
END
${PGM}fs_run load ${W}input || errquit fs_run load

# sort temp index
cat <<END >${W}input
INFILE=${P}temp.tix;
OUTFILE=${P}temp.idx;
PATH=$P;
NSTRING=100000;
NBUF=60;
IOSIZE=300000;
END
${PGM}xfsort ${W}input || errquit xfsort
rm ${P}temp.tix

# build index
cat <<END >${W}input
DATA=$P$DBNAME.d1,$P$DBNAME.d2;
INDEX=$P$DBNAME.dix;
INTNAME=CUSTOMER;
TEMP=${P}temp.idx;
END
${PGM}fs_run index ${W}input || errquit fs_run index
rm ${P}temp.idx
```

For the data-file set, 2 components are assumed to be required. Superfluous components are not created. All files can reside in different file systems (unlike in the example).

Data components require 110% of the input data size. Index construction intermediately requires 30 Bytes and finally at most 14 Bytes per compound.
Indexed Update of Display Files

Indexed update of a display file means that changes to the data files (addition, replacement, or deletion of a compound) cause immediate updates to the corresponding index file. It may be more efficient to use mass update (see below) if only additions are involved. Use a script like:

```
# Update the display files of a customer database
# (no update-enabled users): indexed update

# paths/files/constants
PGM=/xfire/sys/  # program path
W=/xfire/tmp/   # temp path
P=/xfire/db/filesys/  # data path (target file system)
DBNAME=custdb  # database name
INPUT=sdf.dat  # input file name
DEL=delete.lst # deletion list (line: "<RegNo> D")

# error exit
errquit() { echo "*** ERROR in program $*" ; exit 1 ; }

# delete from data file
cat <<END >${W}input
INDEX=$P$DBNAME.dix;
DATA=$P$DBNAME.d1,$P$DBNAME.d2;
INTNAME=CUSTOMER;
OUT=/dev/null;
BRNS=$W$DEL;
END
${PGM}fs_run get ${W}input || errquit fs_run get

# add to data file

 END
${PGM}fs_run iup ${W}input || errquit fs_run iup
```

The lists of data components (keyword DATA) must include additional file names to be created on overflow of the MAXBLOCKS limit specified at file creation time. Sufficient space must be available.
3.10.3.2.6  Mass Update of Display Files

Mass update (only addition possible) of display files means omitting changes to the index when adding compounds to the DATA files. Instead, the index is rebuilt afterwards. Use a script like the following:

```
# Update the display files of a customer database
# (no update-enabled users): mass update

PGM=/xfire/sys/  # program path
W=/xfire/tmp/    # temp path
P=/xfire/db/filesys/  # data path (target file system)
DBNAME=custdb    # database name
INPUT=sdf.da     # input file name

errquit() { echo "*** ERROR in program $*" ; exit 1 ; }

# add to data file
SDF=$W$INPUT;
INDEX=$P$DBNAME.dix;
DATA=$P$DBNAME.d1,$P$DBNAME.d2;
INTNAME=CUSTOMER;
CHECK=YES;
TEMP=${P}temp.tix;

${PGM}fs_run mup ${W}input || errquit fs_run mup

# sort temp index
INFILE=${P}temp.tix;
OUTFILE=${P}temp.idx;
PATH=${P};
NSTRING=100000;
NBUF=60;
IOSIZE=300000;

${PGM}xfsort ${W}input || errquit xfsort
rm ${P}temp.tix

# build index
INDEX=$P$DBNAME.dix;
DATA=$P$DBNAME.d1,$P$DBNAME.d2;
INTNAME=CUSTOMER;
TEMP=${P}temp.idx;

${PGM}fs_run index ${W}input || errquit fs_run index
rm ${P}temp.idx
```

Space estimation and requirements are analogous to the section "Initial loading of display files". The CHECK=YES parameter causes rejection of input RegNos already present in the old data generation. However, uniqueness among input RegNos is not checked.
ERROR MESSAGES OF THE SERVER

The following list of possible errors is sorted by libraries. The first two characters of each error message are defining the library that produced the error.

3.10.3.3 Library CP:

CrossFire Server Error CP_E_LOAD_FILE = -501:
  General failure loading an .INI or .CFG file. Possible reason(s):
  (1) Open failure.
  (2) Read failure.

CrossFire Server Error CP_E_MAIN = -502:
  No information available.

CrossFire Server Error CP_E_SCAN_FILE = -503:
  General failure scanning an .INI or .CFG file. Possible reason(s):
  (1) Name of section too long or section not found.
  (2) Key not found.
  (3) Data buffer exhausted.

CrossFire Server Error CP_E_SELECT_DB = -504:
  General failure to select a database. Possible reason(s):
  (1) Missing or wrong filenames for the database files.

CrossFire Server Error CP_E_SELECT_DATABASE = -505:
  Error selecting a database: the user specific data is inconsistent.
  Possible reason(s):
  (1) Invalid range of registry numbers (e.g. min > max).
  (2) Missing parameters in .xfu-file (e.g. filenames).

CrossFire Server Error CP_E_SEARCH_STRUCT = -506:
  No information available.

CrossFire Server Error CP_E_INIT_SESSION = -507:
  General failure initialising a CROSSFIRE session. Possible reason(s):
  (1) Not enough memory.
  (2) Process ID via function getpid() not available.
  (3) Host ID via function gethostid() not available.
  (4) User ID too long.
  (5) CROSSFIRE.INI file missing or corrupt.

CrossFire Server Error CP_E_INIT_DATABASE = -508:
  General failure to initialise a database. Possible reason(s):
  (1) Not enough memory.
  (2) Wrong database name.

CrossFire Server Error CP_E_INIT_NOSESSION = -509:
  No information available.

CrossFire Server Error CP_E_INIT_NORIGHTS = -510:
  The user has insufficient rights to use the database.

CrossFire Server Error CP_E_LOGFILE_OPEN = -511:
  Cannot open logfile (.XFL-file).

CrossFire Server Error CP_E_LOGFILE_PRINT = -512:
  Cannot write to logfile (.XFL-file).

CrossFire Server Error CP_E_LOGFILE_CLOSE = -513:
  Cannot close logfile (.XFL-file).

CrossFire Server Error CP_E_REJECT_PRGNAME = -514:
  No information available.

CrossFire Server Error CP_E_REJECT_PIPE = -515:
  No information available.

CrossFire Server Error CP_E_REJECT_SEATS = -516:
Login rejected: too many active seats.
CrossFire Server Error CP_E_REJECT_RELOGIN = -517:
  No information available.
CrossFire Server Error CP_E_HITSET_BADPARM = -518:
  bad hitset name
CrossFire Server Error CP_E_HITSET_BADSET = -519:
  bad name or contents of a hitset
CrossFire Server Error CP_E_HITSET_CLEAR = -520:
  error clearing temporary hitsets
CrossFire Server Error CP_E_HITSET_NOMEM = -521:
  no memory for hitset processing
CrossFire Server Error CP_E_HITSET_LOAD = -522:
  error loading the hit numbers of a hitset
CrossFire Server Error CP_E_HITSET_LOADDATA = -523:
  error loading the additional data of a hitset
CrossFire Server Error CP_E_HITSET_BADDATA = -524:
  bad additional data in a hitset
CrossFire Server Error CP_E_HITSET_FORMAT = -525:
  bad hitset file format
CrossFire Server Error CP_E_HITSET_FILEPRESENT = -526:
  hitset to be created already present
CrossFire Server Error CP_E_HITSET_OPEN = -527:
  error opening a hitset file
CrossFire Server Error CP_E_HITSET_IO = -528:
  error reading or writing a hitset file
CrossFire Server Error CP_E_HITSET_INIT = -529:
  error creating a memory hitset
CrossFire Server Error CP_E_HITSET_SAVE = -530:
  error saving the hit numbers of a hitset
CrossFire Server Error CP_E_HITSET_SAVEDATA = -531:
  error saving the additional data of a hitset
CrossFire Server Error CP_E_HITSET_ACCESS = -532:
  error fetching a particular hit number
CrossFire Server Error CP_E_HITSET_MODIFY = -533:
  error updating a hitset
CrossFire Server Error CP_E_HITSET_IMPORT = -582:
  error importing a hitset to the Facts system
CrossFire Server Error CP_E_TYPE_NOMEM = -534:
  no memory for data formatting
CrossFire Server Error CP_E_TYPE_BADPARM = -535:
  bad parameters on the TYPE or SEND command
CrossFire Server Error CP_E_TYPE_GETCT = -536:
  cannot allocate a connection table (no memory)
CrossFire Server Error CP_E_TYPE_OUTPUT = -537:
  error during data formatting for output
CrossFire Server Error CP_E_TYPE_LOADSDF = -538:
  error loading a structure from a SDF file
CrossFire Server Error CP_E_TYPE_USERSET = -539:
  error accessing the user set file
CrossFire Server Error CP_E_TYPE_DELETED = -540:
  attempt to load a deleted structure
CrossFire Server Error CP_E_TYPE_REPORT = -541:
  error performing the REPORT command
CrossFire Server Error CP_E_TYPE_EXPTAB = -553:
error loading SDF expansion table
CrossFire Server Error CP_E_TYPE_EXPAND = -554:
  error expanding a SDF record
CrossFire Server Error CP_E_SEARCH_BADPARM = -542:
  bad parameters on a SEARCH command
CrossFire Server Error CP_E_SEARCH_BADSET = -543:
  invalid hitset specified in a SEARCH command
CrossFire Server Error CP_E_SEARCH_NOMEM = -544:
  out of memory for the SEARCH command
CrossFire Server Error CP_E_SEARCH_COMBINE = -545:
  error logically combining hitsets
CrossFire Server Error CP_E_UPDATE_ILLEGAL = -546:
  the user may not update the current database
CrossFire Server Error CP_E_UPDATE_NOMEM = -547:
  out of memory for update
CrossFire Server Error CP_E_UPDATE_GETCT = -548:
  cannot allocate a connection table (no memory)
CrossFire Server Error CP_E_DELETE_KEY = -549:
  cannot delete keyword
CrossFire Server Error CP_E_INSERT_KEY = -550:
  Cannot insert new entry in configuration file.
CrossFire Server Error CP_E_DELETE_SECTION = -551:
  cannot delete section
CrossFire Server Error CP_E_SAVE_FILE = -552:
  cannot save to a .INI or .XFU file
CrossFire Server Error CP_E_INIT_RETRIEVAL = -580:
  cannot init the retrieval system
CrossFire Server Error CP_E_ACCESS_RETRIEVAL = -581:
  cannot access (use) the retrieval system
CrossFire Server Error CP_E_GETCFDIR = -583:
  cannot download a data structure table

3.10.3.4 Library CT: Connection Table

CrossFire Server Error CT_E_CNV_PTR = -201:
  Internal error setting up memory format. Report to Softron.
CrossFire Server Error CT_E_RING = -202:
  Internal failure of ring detection. Possible reason(s):
  (1) Both "queryFL" and "floadFL" are ON.
CrossFire Server Error CT_E_RING_DUMMY_NOGROUP = -203:
  Internal failure of ring detection:
  Cannot create a dummy atom, because all groups are in use.
CrossFire Server Error CT_E_RING_DUMMY_BONDS = -204:
  Internal failure of ring detection:
  Cannot create a dummy atom: bond list exhausted.
CrossFire Server Error CT_E_RING_CLOS = -205:
  Internal failure of ring detection: too many ring closures.
CrossFire Server Error CT_E_RING_CHAIN_CONFLICT = -206:
  A ring bond must not be marked as a chain bond and a ring
  atom must not be marked as a chain atom.
CrossFire Server Error CT_E_MAKE_INC_LIST = -207:
  Internal error while decoding a bitstring. Report to Softron!
CrossFire Server Error CT_E_DECODE = -208:
  Internal error while decoding a bitstring. Report to Softron!
CrossFire Server Error CT_E_DECODE_ATOMS = -209:
Internal error while decoding a bitstring: too many atoms.
CrossFire Server Error CT_E_DECODE_BONDS = -210:
Internal error while decoding a bitstring: too many bonds.
CrossFire Server Error CT_E_DECODE_FRAGS = -211:
Internal error while decoding a bitstring: too many fragments.
CrossFire Server Error CT_E_DECODE_INCOMPLETE = -212:
Internal error while decoding a bitstring: valency error.
CrossFire Server Error CT_E_DECODE_IXBUILD = -213:
Internal error while decoding a bitstring: increment value > 0x80!
CrossFire Server Error CT_E_ISFS_GLOBAL = -214:
Structure is not a fullstructure due to component attributes.
CrossFire Server Error CT_E_ISFS_NODES = -215:
Structure is not a fullstructure due to node types or node attributes.
CrossFire Server Error CT_E_ISFS_BONDS = -216:
Structure is not a fullstructure due to bond types or bond attributes.
CrossFire Server Error CT_E_ISFS_FRAGS = -217:
Structure is not a fullstructure due to fragment attributes.
CrossFire Server Error CT_E_ISFS_STEREO = -218:
Structure is not a fullstructure due to inconsistent stereo information.
CrossFire Server Error CT_E_MAX_BCH = -219:
Too many bond-reaction-attributes!
CrossFire Server Error CT_E_BCH_BTYPE = -220:
Invalid bond type for a bond change request in a reaction.

3.10.3.5  Library DC:
CrossFire Server Error DC_E_NOMEM = 1:
    No information available.
CrossFire Server Error DC_E_DEFECT = 2:
    No information available.

3.10.3.6  Library QC: Query Compiler
CrossFire Server Error QC_E_CBF_ATOM = -302:
    Invalid atom type or atom attribute in the query.
CrossFire Server Error QC_E_CBF_BOND = -303:
    Invalid bond type or bond attribute in the query.
CrossFire Server Error QC_E_CBF_COMP = -304:
    Error compiling component information. Possible reason(s):
    (1) Invalid value or range for a component attribute.
CrossFire Server Error QC_E_CBF_FRAG = -305:
    Error compiling fragment information. Possible reason(s):
    (1) Fragment information is only allowed for fragments in the
        root structure (not in Markush groups).
    (2) Too many fragments in the structure.
    (3) Invalid value or range for a fragment attribute.
CrossFire Server Error QC_E_CBF_RES = -306:
    Error compiling a Markush group. Possible reason(s):
    (1) Invalid value for the frequency.
    (2) Unexpected start of root structure.
CrossFire Server Error QC_E_SYM_TO_ORD = -307:
    Unknown node symbol in the (query) structure.
CrossFire Server Error QC_E_MAKE_BOND_LIST = -308:
    Error setting up the internal connection table. Possible reason(s):
    (1) Too many bonds in the query.
    (2) Too many free sites.
CrossFire Server Error QC_E_CHECK_GROUP = -309:
Error checking Markush groups. Possible reason(s):
(1) Markush groups must have at least one neighbour or attachment point.
(2) The Markush groups are incorrectly nested.
(3) Inconsistent number of attachment points for multiple occurrences of the same group.
(4) Markush groups with a frequency > 0 must have exactly one attachment point.
(5) Atoms in the root structure must not have attachment points.
(6) An atom has a too high attachment number.
(7) G and G* groups are not allowed in Markush groups. The same applies to unspecified ("empty") Markush groups.
(8) Each fragment ("substituend") in the Markush group must have the same number of attachment points.

CrossFire Server Error QC_E_CHECK_FRAG = -310:
Error checking fragment information. Possible reason(s):
(1) Too many fragments in the query.

CrossFire Server Error QC_E_COMPRESS_CT = -311:
Not used in this program version.

CrossFire Server Error QC_E_HANDLE_HYDRO = -312:
Error checking hydrogens in the query. Possible reason(s):
(1) A hydrogen (or isotope) must not have attachment points.
(2) Hydrogens must be attached with "single" or "any" bonds.
(3) A hydrogen atom must not be attached to an "Also-H"-atom, to a generic group or to a Markush group.

CrossFire Server Error QC_E_FIXUP = -313:
Error during fixup of internal connection table. Possible reason(s):
(1) "Also-H"-atoms must only be attached to at most one atom which in turn must not be an "Also-H"-atom, too!
(2) A generic group must not be attached to another generic group.
(3) A generic group must have at least one neighbour atom. Except for G and G*, it must have exactly one neighbour atom.
(4) The bond type to a generic group must not be of topology "RING" (except for a G* group).
(5) Incorrectly mapped atoms in a reaction:
   a) Both atoms must be the same element.
   b) Both atoms must be "top level" (i.e. not inside a Markush group).
   c) The atoms must NOT be both in a product or educt fragment.

CrossFire Server Error QC_E_PREPARE_STEREO = -314:
Not used in this program version.

CrossFire Server Error QC_E_ATOM_PARITY = -315:
Invalid definition of a stereo tetrahedron. Possible reason(s):
(1) The stereo center must not be a generic or Markush group.
(2) The stereo center must not have attachment points.
(3) The stereo center must have either 3 or 4 neighbor atoms. Otherwise, the parity cannot be computed.
(4) An attached hydrogen atom has a mass value > 3.
(5) The direction of a bond is not clear.
(6) More than one H, D or T is attached to the stereo center.
(7) A stereo center must not be attached to a Markush group.

CrossFire Server Error QC_E_BOND_PARITY = -316:
Invalid definition of a stereo double bond. Possible reason(s):
(1) An end point of the stereo double bond must have at most 3 neighbors and no attachment points. An end point must not
be a generic or Markush group.
(2) Markush groups must not be attached to an end point of a stereo double bond.
(3) An end point must have at least 2 neighbors.
(4) An attached hydrogen atom has a mass value > 3.
(5) More than one H, D or T is attached to an end point.
CrossFire Server Error QC_E_INSERT_ATOM = -317:
An error occurred while inserting a (dummy) atom into the internal connection table. Probably, the bond list is exhausted.
CrossFire Server Error QC_E_CBF_TEXT = -318:
No information available.
CrossFire Server Error QC_E_MEMORY = -319:
Not enough memory to continue.
CrossFire Server Error QC_E_STRUCT_FORMAT = -320:
Invalid format identifier for structure format.
CrossFire Server Error QC_E_WRONG_STERLV_0 = -321:
Stereo level expected but /S0 found. Possible reason:
There are stereo-centers and/or stereo-double bonds in the structure but no stereo-level is specified.
CrossFire Server Error QC_E_WRONG_STERLV_1 = -322:
The wrong stereo level "1" has been specified for the structure:
There are neither stereo double bonds nor stereo tetrahedrons in the structure.
CrossFire Server Error QC_E_WRONG_STERLV_2 = -323:
The wrong stereo level "2" has been specified for the structure:
There are no stereo tetrahedrons in the structure.
CrossFire Server Error QC_E_UNKNOWN_STERLV = -324:
An unknown stereo level has been specified for the structure.
Supported stereo levels are /S0, /S1 and /S2.
CrossFire Server Error QC_E_RXN_FORMAT = -325:
Unknown format for reaction scanner.
CrossFire Server Error QC_E_CBF_MAX_REACTANT = -326:
Too many reactants in reaction.
CrossFire Server Error QC_E_CBF_REACTANT = -327:
Internal error in call-back-function qc_cbf_reactant().
CrossFire Server Error QC_E_CBF_ROLE_MISSING = -328:
Each reactant must have a specified role.
CrossFire Server Error QC_E_CBF_REACTANT_NUMBER = -329:
Reactand index larger than maximum number of reactants.
CrossFire Server Error QC_E_CBF_SAD = -330:
Error scanning SAD string.
CrossFire Server Error QC_E_CBF_SAD_MEM = -331:
Not enough memory to allocate tmp. Rosdal-string while scanning SAD format.
CrossFire Server Error QC_E_CBF_RXDIR = -332:
Invalid keyword for "direction" of reaction.
CrossFire Server Error QC_E_MOVE_ATOM = -333:
Internal error while moving atoms: size of CT exhausted.
CrossFire Server Error QC_E_CBF_ATOM_FRAGNO = -334:
The same atom index was found in different fragments.
CrossFire Server Error QC_E_CBF_REGCT = -335:
Error posting registration-CT to CROSSFIRE-CT.
3.10.3.7 Library AB: ABAS
CrossFire Server Error AB_E_GENER = -2102:
   general (unspecified) error
CrossFire Server Error AB_E_GETCT = -2103:
   cannot allocate connection table
CrossFire Server Error AB_E_GETBT = -2104:
   cannot allocate storage for backtracking list
CrossFire Server Error AB_E_QUERY = -2105:
   error translating query
CrossFire Server Error AB_E_ABINIT = -2106:
   ABAS init error: no memory or bad state of module
CrossFire Server Error AB_E_ABAS = -2107:
   error during ABAS processing
CrossFire Server Error AB_E_IO = -2108:
   file open or read error during ABAS
1 AB_E_BREAK
CrossFire Server Error DC_E_NOMEM = 1:
   No information available.
10 AB_E_BADINIT
CrossFire Server Error AB_E_BADINIT = 10:
   bad initialization state of the ABAS module
11 AB_E_NOMEM
CrossFire Server Error AB_E_NOMEM = 11:
   ABAS: out of memory
12 AB_E_RINGS
CrossFire Server Error AB_E_RINGS = 12:
   ABAS: The current full structure contains too many rings.
13 AB_E_TREEMEM
CrossFire Server Error AB_E_TREEMEM = 13:
   overflow of backtracking list
14 AB_E_TREEOVF
CrossFire Server Error AB_E_TREEOVF = 14:
   overflow of backtracking list
15 AB_E_STARTATOM
CrossFire Server Error AB_E_STARTATOM = 15:
   ABAS: unable to find a proper starting atom
16 AB_E_PATH
CrossFire Server Error AB_E_PATH = 16:
   ABAS: unable to find a path through the query structure
17 AB_E_ATTACH
CrossFire Server Error AB_E_ATTACH = 17:
   ABAS: inconsistent attachment points
18 AB_E_FINDATT
CrossFire Server Error AB_E_FINDATT = 18:
   ABAS: inconsistent attachment points
19 AB_E_TRATOM
CrossFire Server Error AB_E_TRATOM = 19:
   ABAS: error processing normal atom
20 AB_E_TRREST
CrossFire Server Error AB_E_TRREST = 20:
   ABAS: error processing Markush node

3.10.3.8 Library RF: Reaction processing
CrossFire Server Error RF_E_GENER = -4101:
general (unspecified) error
CrossFire Server Error RF_E_NOMEM = -4102:
out of memory
CrossFire Server Error RF_E_FRAME_SAD = -4103:
invalid frame <SAD...>SAD
CrossFire Server Error RF_E_FRAME_RXN = -4104:
invalid frame <RXN...>RXN
CrossFire Server Error RF_E_FRAME_STR = -4105:
invalid frame <STR...>STR
CrossFire Server Error RF_E_KEYWORD = -4106:
invalid keyword format or data
CrossFire Server Error RF_E_MAP1 = -4111:
incorrect mapping found during scan.
CrossFire Server Error RF_E_MAP2 = -4112:
incorrect mapping found during scan.
CrossFire Server Error RF_E_MAP3 = -4113:
incorrect mapping found during scan.
CrossFire Server Error RF_E_MAP4 = -4114:
incorrect mapping found during scan.
CrossFire Server Error RF_E_MAP5 = -4115:
incorrect mapping found during scan.
CrossFire Server Error RF_E_BADDATA = -4116:
data invalid for reaction display.
CrossFire Server Error RF_E_OVERSIZED = -4117:
caller buffer is too small.
CrossFire Server Error RF_E_PACK = -4118:
error introducing packed atom numbering.
CrossFire Server Error RF_E_SCALE = -4120:
error during coordinate scaling.
CrossFire Server Error RF_E_SCANSDF1 = -4121:
No information available.
CrossFire Server Error RF_E_SCANSDF2 = -4122:
No information available.
CrossFire Server Error RF_E_SCANSDF3 = -4123:
No information available.
CrossFire Server Error RF_E_SCANSDF4 = -4124:
No information available.
CrossFire Server Error RF_E_SCANSDF5 = -4125:
No information available.
CrossFire Server Error RF_E_SCANSDF6 = -4126:
No information available.
CrossFire Server Error RF_E_SCANSDF7 = -4127:
No information available.
CrossFire Server Error RF_E_SCANSDF8 = -4128:
No information available.
CrossFire Server Error RF_E_SCANSDF9 = -4129:
No information available.
CrossFire Server Error RF_E_SCANSDF10 = -4130:
No information available.
CrossFire Server Error RF_E_SCANSDF11 = -4131:
No information available.
CrossFire Server Error RF_E_SCANSDF12 = -4132:
No information available.
CrossFire Server Error RF_E_SCANSDF13 = -4133:
CrossFire Server Error RF_E_SCANSDF14 = -4134:
No information available.
CrossFire Server Error RF_E_SCANSDF15 = -4135:
No information available.
CrossFire Server Error RF_E_SCANSDF16 = -4136:
error scanning a reaction in SDF format.
CrossFire Server Error RF_E_CENTERS = -4140:
error detecting reaction centers.
CrossFire Server Error RF_E_FIX1 = -4141:
No information available.
CrossFire Server Error RF_E_FIX2 = -4142:
No information available.
CrossFire Server Error RF_E_FIX3 = -4143:
No information available.
CrossFire Server Error RF_E_FIX4 = -4144:
No information available.
CrossFire Server Error RF_E_FIX5 = -4145:
No information available.
CrossFire Server Error RF_E_FIX6 = -4146:
No information available.
CrossFire Server Error RF_E_FIX7 = -4147:
No information available.
CrossFire Server Error RF_E_FIX8 = -4148:
No information available.
CrossFire Server Error RF_E_FIX9 = -4149:
No information available.
CrossFire Server Error RF_E_FIX10 = -4150:
No information available.
CrossFire Server Error RF_E_FIX11 = -4151:
No information available.
CrossFire Server Error RF_E_FIX12 = -4152:
No information available.
CrossFire Server Error RF_E_FIX13 = -4153:
No information available.
CrossFire Server Error RF_E_FIX14 = -4154:
No information available.
CrossFire Server Error RF_E_FIX15 = -4155:
No information available.
CrossFire Server Error RF_E_FIX16 = -4156:
error fixing up SDF record.
CrossFire Server Error RF_E_SADPARAM = -4160:
bad parameters calling SAD access function
CrossFire Server Error RF_E_SADACCESS = -4161:
invalid SAD object
CrossFire Server Error RF_E_HILITE = -4162:
out of memory when hiliting atoms

3.10.3.9 Library SC: Screening
CrossFire Server Error SC_E_MAIN = -701:
Internal general error in the screening,
e.g. not yet implemented features.
CrossFire Server Error SC_E_TREE = -705:
Internal failure setting up the backtracking tree for the
screening. Please, report the trouble causing query to Softron.

CrossFire Server Error SC_E_START_ATOM = -706:
The screening cannot find a feasible starting atom.
Possible reason: No regular atom in the query.

CrossFire Server Error SC_E_SWAP_PUT = -707:
Error writing to the temporary swap file.

CrossFire Server Error SC_E_SWAP_GET = -708:
Error reading from the temporary swap file.

CrossFire Server Error SC_E_SWAP_OPEN = -709:
Error opening the temporary swap file.

CrossFire Server Error SC_E_SWAP_CREATE = -710:
Error creating the temporary swap file.

CrossFire Server Error SC_E_SWAP_CLOSE = -711:
Error closing the temporary swap file.

CrossFire Server Error SC_E_SWAP_RESET = -712:
Error resetting the temporary swap file.

CrossFire Server Error SC_E_SWAP_REWRITE = -713:
Error rewriting the temporary swap file.

CrossFire Server Error SC_E_SWAP_INIT = -714:
No information available.

CrossFire Server Error SC_E_MAP_PUT = -715:
No information available.

CrossFire Server Error SC_E_MAP_GET = -716:
No information available.

CrossFire Server Error SC_E_SHOW = -717:
No information available.

CrossFire Server Error SC_E_DECO = -718:
Error decoding the current bitstring.

CrossFire Server Error SC_E_TREE_USE_GROUP = -719:
The screening failed to set up the backtracking list for the
current query because of Markush groups in the structure. This
is an internal error which should be reported to Softron.

CrossFire Server Error SC_E_TREE_COPY_GROUP = -720:
The screening failed to set up the backtracking list for the
current query because of Markush groups in the structure. This
is an internal error which should be reported to Softron.

CrossFire Server Error SC_E_BREAK = -721:
The screening has encountered a break request of the user
and has terminated without a final result.

CrossFire Server Error SC_E_INIT = -722:
No information available.

CrossFire Server Error SC_E_TREE_NGROUP = -723:
Too many Markush groups in the query. There are either too many
different groups or too many occurrences of the same group.

CrossFire Server Error SC_E_TREE_NATOMS = -724:
Too many atoms in the structure for the screening. This may be
due to many free-sites or due to a lot of occurrences of a Markush
group.

CrossFire Server Error SC_E_TREE_NO_MORE_STARTATOMS = -725:
No more startatoms available. Screening terminated normally.

CrossFire Server Error SC_E_SELECT_START_ATOM = -726:
Error selecting start-atom for the screening.

CrossFire Server Error SC_E_SEEK_TREE = -727:
Error during seek operation on tree-file.
CrossFire Server Error SC_E_READ_TREE = -728:
Error during read operation on tree-file.

CrossFire Server Error SC_E_MEMORY = -729:
Memory allocation for connection tables failed in screening.

3.10.3.10 Library IX: Indexing

CrossFire Server Error IX_E_CREATE_TREE = -601:
General failure creating complete index tree.

CrossFire Server Error IX_E_CLOSE_TREE = -602:
General failure closing complete index tree.

CrossFire Server Error IX_E_CREATE_FILE = -603:
General failure creating an index tree file. Possible reason(s):
(1) No memory to allocate file buffers.
(2) Error writing the header block(s) to the file.

CrossFire Server Error IX_E_CLOSE_FILE = -604:
General failure closing tree-file.

CrossFire Server Error IX_E_STORE_TREE = -605:
General failure writing to index tree. Possible reason(s):
(1) Data record too long (internal error).
(2) Wrong address code (internal error).
Please, report to Softron!

CrossFire Server Error IX_E_END_STORE_TREE = -606:
Error while flushing the file buffers.

CrossFire Server Error IX_E_BUILD = -607:
General failure creating the index tree.

CrossFire Server Error IX_E_PARAMETERS = -608:
Invalid parameters in configuration file.

CrossFire Server Error IX_E_OPEN_FILE = -609:
General failure opening tree-file.

CrossFire Server Error IX_E_OPEN_TREE = -610:
General failure opening complete index tree.

CrossFire Server Error IX_E_READ_BUNDLE = -611:
General failure reading from index tree file.

CrossFire Server Error IX_E_READ_TREE = -612:
General failure reading the index tree.

CrossFire Server Error IX_E_READ_TREE_POINTER = -613:
Internal error reading index tree. Possible reason: incompatible tree-files!

CrossFire Server Error IX_E_OPEN_BUNDLE = -614:
General failure opening tree file. Possible reason: the file buffer cannot be allocated.

CrossFire Server Error IX_E_CLOSE_BUNDLE = -615:
Error closing tree file.

CrossFire Server Error IX_E_GET_TREE_NAME = -616:
Error creating name for tree-file. Possible reason: the filename is too long or is not available.

CrossFire Server Error IX_E_MAKE = -617:
Internal error generating TREE-data. Please, report to Softron.

CrossFire Server Error IX_E_HEADER_SIZE = -618:
Incompatible size of tree-header! Tree-files are not compatible with current program version.

CrossFire Server Error IX_E_READ_ADRLEN = -619:
Internal error reading bitstring: adr_len > 4 !
Please, report to Softron!
CrossFire Server Error IX_E_REOPEN_FILE = -620:
Error re-opening a tree-file.
CrossFire Server Error IX_E_FREE_HANDLE = -621:
Error freeing the file handle of a tree-file.
CrossFire Server Error IX_E_STAT_READ_TREE = -622:
Error reading statistics from tree-file.
CrossFire Server Error IX_E_STAT_INIT = -623:
Error allocating memory for statistics.
CrossFire Server Error IX_E_STAT_DUMP = -624:
Error dumping statistics to file.
CrossFire Server Error IX_E_STAT_READ = -625:
Error reading statistics from binary file.
CrossFire Server Error IX_E_PATCH = -626:
Error adding statistics to index tree.

3.10.3.11 Library ER:
CrossFire Server Error ER_E_TXTFILE_OPEN = -3001:
Cannot open text file with error messages.

3.10.3.12 Library ST: Stereo
CrossFire Server Error ST_E_ATOM_PARITY = -401:
Parity of stereo tetrahedron cannot be evaluated.
CrossFire Server Error ST_E_BOND_PARITY = -402:
Parity of stereo double bond cannot be evaluated. Possible reason(s):
(1) No or missing coordinates for relevant atoms.
(2) Ambiguous input of ligand bond(s) (e.g. wrong direction).
(3) Ligand bond (nearly) collinear with stereo double bond.

3.10.3.13 Library FS: Filesystem
CrossFire Server Error FS_E_CREATE = -2203:
data file creation error: file may already exist
CrossFire Server Error FS_E_FINISH = -2204:
error finishing access to a database
CrossFire Server Error FS_E_OPEN = -2205:
error opening a database
CrossFire Server Error FS_E_WRITE = -2206:
error writing a member to EOF
CrossFire Server Error FS_E_READ = -2207:
error reading members in physical sequence
CrossFire Server Error FS_E_INDEX = -2208:
error creating or accessing the index
CrossFire Server Error FS_E_GET = -2209:
error getting a member by direct access
CrossFire Server Error FS_E_TEST = -2210:
error testing for member existence
CrossFire Server Error FS_E_PUT = -2211:
error adding or replacing a member
CrossFire Server Error FS_E_DELETE = -2212:
error deleting a member
CrossFire Server Error FS_E_EXTEND = -2213:
error extending the data component by mass update
CrossFire Server Error FS_E_NOMEM = -2299:
out of memory
CrossFire Server Error FS_E_MAXBLOCKS = -2221:
bad parameter MAXBLOCKS
CrossFire Server Error FS_E_BLOCKSIZE = -2222:
bad parameter BLOCKSIZE
CrossFire Server Error FS_E_INTNAME = -2223:
bad parameter for the internal name
CrossFire Server Error FS_E_MAKEPRIME = -2224:
cannot create the prime data component header
CrossFire Server Error FS_E_NEWTEMP = -2225:
error creating a temporary index file
CrossFire Server Error FS_E_FINHEADER = -2226:
error finishing a data file header block
CrossFire Server Error FS_E_ACCESSPRIME = -2227:
error interpreting the prime data component header
CrossFire Server Error FS_E_CREATETEMP = -2228:
error creating a temporary index file
CrossFire Server Error FS_E_OLDTEMP = -2229:
error opening an existing temporary index file
CrossFire Server Error FS_E_ACCESSFINAL = -2230:
error accessing the final data component
CrossFire Server Error FS_E_SEEKFINAL = -2231:
error seeking to the active output position
CrossFire Server Error FS_E_MEMBLEN = -2232:
invalid member length
CrossFire Server Error FS_E_MEMBREAD = -2233:
error reading member
CrossFire Server Error FS_E_BADMEMBER = -2234:
bad member data format
CrossFire Server Error FS_E_PROVIDEBLOCK = -2235:
cannot provide a new data block
CrossFire Server Error FS_E_MEMBWRITE = -2236:
error writing a member
CrossFire Server Error FS_E_TEMPWRITE = -2237:
error writing to a temp. index file
CrossFire Server Error FS_E_GETLOCATE = -2238:
cannot locate a member in the index
CrossFire Server Error FS_E_GETLOADBLOCK = -2239:
error loading the data block with the actual member
CrossFire Server Error FS_E_GETEXTRACT = -2240:
error extracting a member from its data block
CrossFire Server Error FS_E_STAGES = -2241:
too many index stages - capacity exceeded
CrossFire Server Error FS_E_INTHDRWRITE = -2242:
error (re-)writing the index header
CrossFire Server Error FS_E_TEMPREAD = -2243:
error reading from the temp. index file
CrossFire Server Error FS_E_INDFLUSH = -2244:
error finishing index file building
CrossFire Server Error FS_E_SORTORDER = -2245:
A temporary index file was not properly sorted or
contains duplicate member key numbers.
CrossFire Server Error FS_E_BADMODE = -2246:
bad file access mode specified
CrossFire Server Error FS_E_INDMEMORY = -2247:
no memory for index creation or access
CrossFire Server Error FS_E_NAMEMATCH = -2249:
The internal name specified does not match its counterpart defined for the actual database.

CrossFire Server Error FS_ESEEKDATA = -2250:
error seeking to a data file block

CrossFire Server Error FS_E_WALKFILE = -2251:
index file inconsistency detected

CrossFire Server Error FS_E_WALKMEM = -2252:
index file inconsistency detected

CrossFire Server Error FS_E_WALKLOAD1 = -2253:
index file inconsistency detected

CrossFire Server Error FS_E_WALKHDR = -2254:
index file inconsistency detected

CrossFire Server Error FS_E_WALKWEIGHT1 = -2255:
index file inconsistency detected

CrossFire Server Error FS_E_WALKSORTORDER = -2256:
index file inconsistency detected

CrossFire Server Error FS_E_WALKWEIGHT2 = -2257:
index file inconsistency detected

CrossFire Server Error FS_E_WALKSORTORD1 = -2258:
index file inconsistency detected

CrossFire Server Error FS_E_WALKDOWNLINK1 = -2259:
index file inconsistency detected

CrossFire Server Error FS_E_WALKLOAD2 = -2260:
index file inconsistency detected

CrossFire Server Error FS_E_WALKBACKLINK1 = -2261:
index file inconsistency detected

CrossFire Server Error FS_E_WALKLOAD3 = -2262:
index file inconsistency detected

CrossFire Server Error FS_E_WALKBACKLINK2 = -2263:
index file inconsistency detected

CrossFire Server Error FS_E_WALKWEIGHT3 = -2264:
index file inconsistency detected

CrossFire Server Error FS_E_WALKTAIL = -2265:
index file inconsistency detected

CrossFire Server Error FS_E_SUPERFLUOUSPTRS = -2266:
index file inconsistency detected

CrossFire Server Error FS_E_WALKLOAD4 = -2267:
index file inconsistency detected

CrossFire Server Error FS_E_WALKBADCOUNT = -2268:
index file inconsistency detected

CrossFire Server Error FS_E_WALKSORTORD2 = -2269:
index file inconsistency detected

CrossFire Server Error FS_E_WALKDOWNLINK2 = -2270:
index file inconsistency detected

CrossFire Server Error FS_E_WALKLOAD5 = -2271:
index file inconsistency detected

CrossFire Server Error FS_E_WALKBACKLINK3 = -2272:
index file inconsistency detected

CrossFire Server Error FS_E_WALKFORWLINK = -2273:
index file inconsistency detected

CrossFire Server Error FS_E_WALKLOAD6 = -2274:
index file inconsistency detected

CrossFire Server Error FS_E_WALKBACKLINK4 = -2275:
index file inconsistency detected
CrossFire Server Error FS_E_WALKWEIGHT4 = -2276:
index file inconsistency detected
CrossFire Server Error FS_E_WALKBADSIZE = -2277:
index file inconsistency detected
CrossFire Server Error FS_E_WALKLOAD7 = -2278:
index file inconsistency detected
CrossFire Server Error FS_E_WALKBADCHAIN = -2279:
index file inconsistency detected
CrossFire Server Error FS_E_LOADBLOCK = -2280:
unable to load a data or index block
CrossFire Server Error FS_E_DUPMEMBER = -2281:
duplicate member key number detected
CrossFire Server Error FS_E_NOMEMBER = -2282:
member to be replaced not found in data block
CrossFire Server Error FS_E_SAVEBLOCK = -2283:
unable to save a data or index block
CrossFire Server Error FS_E_BADKEY = -2284:
member key number out of range
CrossFire Server Error FS_E_CHSIZE = -2285:
error truncating the index file
CrossFire Server Error FS_E_REOPEN = -2286:
error reopening a file
CrossFire Server Error FS_E_NEWBLOCK = -2287:
request for a new data or index block fails
CrossFire Server Error FS_E_FILEEXIST = -2288:
file to be created already exists
CrossFire Server Error FS_E_NEWDATA = -2289:
cannot create a data file component
CrossFire Server Error FS_E_DATHDRWRITE = -2290:
error writing a data component header
CrossFire Server Error FS_E_BADNAME = -2291:
bad parameter specified
CrossFire Server Error FS_E_DATHDRREAD = -2292:
error reading a data component header
CrossFire Server Error FS_E_COUNTMATCH = -2293:
bad file sequence number for the actual data component
CrossFire Server Error FS_E_BADTEMP = -2294:
file name too long
CrossFire Server Error FS_E_INDHDRWRITE = -2295:
error writing the index file header
CrossFire Server Error FS_E_INDOPEN = -2296:
error opening the index file
CrossFire Server Error FS_E_BADTEMP = -2297:
error opening a temporary index file

3.10.3.14 Library RS: Rosdal Scanner
CrossFire Server Error RS_E_INTERNAL_ERROR = -1001:
Internal error. Report to Softron! Please, provide
the erroneous (query) structure!
CrossFire Server Error RS_E_UNEXPECTED_END = -1002:
Unexpected end of ROSDAL string.
CrossFire Server Error RS_E_INVALID_WORK_POINTER = -1003:
Internal error. Report to Softron!
CrossFire Server Error RS_E_UNKNOWN_SYNTAX = -1004:
General syntax error.
CrossFire Server Error RS_E_INTEGER_VALUE = -1005:
Invalid inter value.
CrossFire Server Error RS_E_BOND_SYMBOL = -1006:
Invalid bond symbol.
CrossFire Server Error RS_E_NODE_SPEC = -1007:
Invalid atom attribute found.
CrossFire Server Error RS_E_NODE_SYMBOL = -1008:
Invalid node symbol found.
CrossFire Server Error RS_E_BOND = -1009:
Incorrect bond found. Possible reason(s):
(1) An atom cannot be connected to itself.
(2) "EXACT"-flag for shortcut bond sequence not allowed.
CrossFire Server Error RS_E_RANGE = -1010:
Incorrect range for component attributes.
CrossFire Server Error RS_E_COMMENT = -1011:
Incorrect syntax for 'wild' comment: %% <comment> %%.
CrossFire Server Error RS_E_GROUP = -1012:
Incorrect syntax for Markush group.
CrossFire Server Error RS_E_FREQUENCY = -1013:
Syntax error for frequency of a Markush group.
CrossFire Server Error RS_E_DOUBLE_VALUE = -1014:
No information available.
CrossFire Server Error RS_E_HEX_CRD = -1015:
Error scanning hex coordinates.
CrossFire Server Error RS_E_MAX_SYMBOL_LEN = -1016:
No information available.
CrossFire Server Error RS_E_SITE_NUMBERS = -1017:
Incorrect or more than 2 site-numbers at an atom found.
A site number must be in the range 1..9.
CrossFire Server Error RS_E_CUT_STR = -1018:
No information available.
CrossFire Server Error RS_E_TYPE = -1019:
No information available.
CrossFire Server Error RS_E_MOD = -1020:
Invalid "modification" value found.
CrossFire Server Error RS_E_CPERC = -1021:
No information available.
CrossFire Server Error RS_E_COEFF = -1022:
Invalid "fragment coefficient" value found.
CrossFire Server Error RS_E_INVALID_KEY = -1023:
No information available.
CrossFire Server Error RS_E_PARITY = -1024:
Error scanning stereo information.
CrossFire Server Error RS_E_PTYPE = -1025:
No information available.
CrossFire Server Error RS_E_INVALID_STVEC = -1026:
No information available.
CrossFire Server Error RS_E_INTERNAL_ERROR = -1001:
Internal error. Report to Softron! Please, provide the erroneous (query) structure!

3.10.3.15 Library SD: SDF Scanner
CrossFire Server Error SD_E_NOMEM = -2098:
out of memory in the SDF scanner
CrossFire Server Error SD_E_DEFECT = -2099:
The actual SDF record to be scanned does not meet
the SDF format specifications.
CrossFire Server Error SD_E_INTERFACE = -2001:
bad callback function pointers calling the SDF scanner
CrossFire Server Error SD_E_LISTLEN = -2002:
improper value for the length of an SDF list
CrossFire Server Error SD_E_SYSTEM = -2003:
error scanning a particular SDF list: SYSTEM
CrossFire Server Error SD_E_MULTIFRAG = -2004:
error scanning a particular SDF list: MULTIFRAGMENT
CrossFire Server Error SD_E_IT = -2005:
error scanning a particular SDF list: IST
CrossFire Server Error SD_E_BRCT_GEN = -2006:
error scanning a particular SDF list: BRCT
CrossFire Server Error SD_E_FETCHLIST = -2007:
error locating an SDF list
CrossFire Server Error SD_E_FROMLIST = -2008:
error scanning a particular SDF list: from list
CrossFire Server Error SD_E_RCLIST = -2009:
error scanning a particular SDF list: ring closures
CrossFire Server Error SD_EATYPE = -2010:
error scanning a particular SDF list: atomic numbers
CrossFire Server Error SD_E_LH = -2028:
error scanning a particular SDF list: H counts
CrossFire Server Error SD_E_STER_AS = -2011:
error scanning a particular SDF list: atom stereo
CrossFire Server Error SD_E_STER_BS = -2012:
error scanning a particular SDF list: bond stereo
CrossFire Server Error SD_E_VA = -2013:
error scanning a particular SDF list: axis stereo
CrossFire Server Error SD_E_LC = -2014:
error scanning a particular SDF list: localized charge
CrossFire Server Error SD_E_DC = -2015:
error scanning a particular SDF list: deloc. charge
CrossFire Server Error SD_E_LR = -2016:
error scanning a particular SDF list: loc. radical
CrossFire Server Error SD_E_MA = -2017:
error scanning a particular SDF list: isotopic mass
CrossFire Server Error SD_E_STER_PA = -2018:
error scanning a particular SDF list: stereo polyhedron
CrossFire Server Error SD_E_AG = -2019:
error scanning a particular SDF list: graph atom coords.
CrossFire Server Error SD_E_BG = -2020:
error scanning a particular SDF list: graph bond orient.
CrossFire Server Error SD_E_NG = -2021:
error scanning a particular SDF list: nongraph atom coords.
CrossFire Server Error SD_E_BO = -2022:
error scanning a particular SDF list: bond orders
CrossFire Server Error SD_E_ZG = -2023:
error scanning a particular SDF list: graph z coords.
CrossFire Server Error SD_E_ZN = -2024:
error scanning a particular SDF list: nongraph z coords.
CrossFire Server Error SD_E_MODT = -2025:
  error scanning a particular SDF list: modification text
CrossFire Server Error SD_E_TM = -2026:
  error scanning a particular SDF list: tautomeric groups
CrossFire Server Error SD_E_TREE = -2027:
  error analyzing the total SDF record
CrossFire Server Error SD_ESTER_XS = -2029:
  error scanning a particular SDF list: conventional axes
CrossFire Server Error SD_ESTER_PB = -2030:
  error scanning a particular SDF list: extended bonds
CrossFire Server Error SD_ESTER_PX = -2031:
  error scanning a particular SDF list: extended axes
CrossFire Server Error SD_E_NS = -2032:
  error scanning a particular SDF list: descriptors
CrossFire Server Error SD_E_SD = -2033:
  error scanning a particular SDF list: descriptors
CrossFire Server Error SD_E_OS = -2034:
  error scanning a particular SDF list: descriptors
CrossFire Server Error SD_E_CA = -2035:
  error scanning a particular SDF list: CIP atom parity
CrossFire Server Error SD_E_CB = -2036:
  error scanning a particular SDF list: CIP bond parity
CrossFire Server Error SD_E_CX = -2037:
  error scanning a particular SDF list: CIP axis parity
CrossFire Server Error SD_E_DF = -2038:
  error scanning a particular SDF list: display formula

3.10.3.16 Library BT:
CrossFire Server Error BT_E_BADBLKSIZE = -2301:
  bad blocksize read or specified
CrossFire Server Error BT_E_BADFINISH = -2302:
  cannot finish file
CrossFire Server Error BT_E_BADPARM = -2303:
  bad caller parameter
CrossFire Server Error BT_E_FILETAB = -2304:
  error storing file table to search header
CrossFire Server Error BT_E_INDCREATE = -2305:
  cannot create index file
CrossFire Server Error BT_E_INDFIRST = -2306:
  error writing first index block
CrossFire Server Error BT_E_INDFULL = -2307:
  first index block is full
CrossFire Server Error BT_E_INDMEM = -2308:
  no memory for index buffers
CrossFire Server Error BT_E_INDOPEN = -2309:
  cannot open index file
CrossFire Server Error BT_E_INDPEEK = -2310:
  cannot read in index blocksize
CrossFire Server Error BT_E_INDREAD = -2311:
  error reading index block
CrossFire Server Error BT_E_INDREWIND = -2312:
  error rewinding index
CrossFire Server Error BT_E_INDTREE = -2313:
  error building binary tree on index block
CrossFire Server Error BT_E_INDBLOCK = -2314:
  error writing index block
CrossFire Server Error BT_E_INDFIRST = -2315:
  error writing 1st index block
CrossFire Server Error BT_E_INDDAPPEND = -2328:
  error appending intermediate block to the main index
CrossFire Server Error BT_E_MAXLEN = -2316:
  bitstring too long
CrossFire Server Error BT_E_MINLEN = -2317:
  bitstring too short
CrossFire Server Error BT_E_PHYSEOF = -2318:
  physical EOF on search without logical EOF
CrossFire Server Error BT_E_REPCOUNT = -2319:
  bad repetition count for bitstring
CrossFire Server Error BT_E_SORTORDER = -2320:
  bad bitstring sort order
CrossFire Server Error BT_E_SRCCREATE = -2321:
  cannot create search file
CrossFire Server Error BT_E_SRCMEM = -2322:
  no memory for search buffers
CrossFire Server Error BT_E_SRCCOM = -2323:
  cannot open search file
CrossFire Server Error BT_E_SRCREAD = -2324:
  error reading search block
CrossFire Server Error BT_E_SRCWBLOCK = -2325:
  error writing search block
CrossFire Server Error BT_E_SRCWFIRST = -2326:
  error writing 1st search block
CrossFire Server Error BT_E_SWITCHFILE = -2327:
  error switching to next file partition

3.10.3.17  Library CU: Database maintenance
CrossFire Server Error CU_E_INIT = -4001:
  Error initialising program. Probably memory exhausted.
CrossFire Server Error CU_E_WRITE_CFG = -4002:
  Error writing to configuration file.
CrossFire Server Error CU_E_COLL_MAIN = -4010:
  General program failure.
CrossFire Server Error CU_E_UPD_MAIN = -4020:
  General program failure.
CrossFire Server Error CU_E_DBNEW_MAIN = -4030:
  General program failure.
CrossFire Server Error CU_E_USER_MAIN = -4040:
  General program failure.
CrossFire Server Error CU_E_USER_LIST = -4041:
  No information available.
CrossFire Server Error CU_E_USER_ADD = -4042:
  No information available.
CrossFire Server Error CU_E_USER_DEL = -4043:
  No information available.
CrossFire Server Error CU_E_FSYS = -4050:
  Filesystem error.
CrossFire Server Error CU_E_SAVE = -4051:
  Error saving to INI file.
CrossFire Server Error CU_E_DBTAB = -4052:
  Database table setup error.
CrossFire Server Error CU_E_LOAD = -4053:
  Error loading from INI file.
CrossFire Server Error CU_E_LOADCTL = -4054:
  Error in load control program.

3.10.3.18    Library UT: Utilities
CrossFire Server Error UT_E_EXPIRED = -901:
  The current program version has expired. Please, contact
  Softron!
CrossFire Server Error UT_E_SEFILE_OPEN = -902:
  Error opening SE structure file (ROSDAL file).
CrossFire Server Error UT_E_SEFILE_READ = -903:
  No information available.
CrossFire Server Error UT_E_SEFILE_FORMAT = -904:
  No information available.
CrossFire Server Error UT_E_SEFILE_MAX_ROSDAL = -905:
  No information available.
CrossFire Server Error UT_E_LIC_MAKE = -906:
  Error creating an CROSSFIRE license string.
CrossFire Server Error UT_E_LIC_MAKE_PARMS = -907:
  Creating an CROSSFIRE license string:
  Wrong parameters for function ut_LicMake().
CrossFire Server Error UT_E_LIC_MAKE_INVALID_PRODUCT = -908:
  Creating an CROSSFIRE license string:
  Invalid product shortkey.
CrossFire Server Error UT_E_LIC_MAKE_INVALID_DATE = -909:
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  Invalid date (e.g. format, before 1.1.94).
CrossFire Server Error UT_E_LIC_SCAN = -910:
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  Invalid product shortkey.
CrossFire Server Error UT_E_LIC_PARSE = -913:
  Error parsing CROSSFIRE licenses (e.g. wrong license strings).
CrossFire Server Error UT_E_VERIFY_MONOTONY = -914:
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