

# **CSDS Release and Installation Notes**

## **2012 Release**

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## 1. CSD System Release Package

The CSD System release is distributed annually. The 2012 release contains:

- The Cambridge Structural Database, Version 5.33
- Access to WebCSD (unlimited site licence holders only)
- ConQuest 1.14 for Linux, Windows and Mac OS X (including Classroom ConQuest)
- Mercury 3.0 for Linux, Windows and Mac OS X
- IsoStar 2.1.3 for Linux (server and client) and IsoStar 2.1.3 PC and Mac OS X clients
- Mogul 1.4 for Linux, Windows and Mac OS X
- PreQuest for Linux, Windows and Mac OS X
- SuperStar 2.0.3 for Linux and Windows (academic licence holders only. Available as an upgrade for industrial users).
- DASH 3.3 for Windows (academic licence holders only. Available as an upgrade for industrial users)
- Printed Newsletter, What's New, and Quick Install guides

Supported platforms are listed elsewhere (see Section Supported Platforms, page 4).

The 2012 release of the CSD System is supplied on three or four DVD-ROMs depending on what your licence gives you access to:

### ***Windows DVD***

- ConQuest 1.14, Mercury 3.0, PreQuest, Mogul 1.4 and IsoStar 2.1.3 PC Client.
- All CSD and Mogul data files.

### ***Linux DVD***

- ConQuest 1.14, Mercury 3.0, PreQuest, Mogul 1.4, IsoStar 2.1.3 Client for Linux.
- IsoStar 2.1.3 data and server software for Linux.
- All database files for Linux.

### ***Mac OS X DVD***

- ConQuest 1.14, Mercury 3.0, Vista, PreQuest, Mogul 1.4 and IsoStar 2.1.3 Client.
- All database files.

### ***SuperStar & DASH DVD***

- A fourth DVD for installing SuperStar and DASH is also available to academic licence holders.

## 2. Database Content and Information

- The number of CSD entries in the 2012 release of the CSD System is 577,833.
- The database will expire on 31st March 2013.

## 3. What's New

### Polymorphism risk assessment

- A new Solid Form Informatics tool is available as part of the CSD Solid Form module (previously known as the Materials module of Mercury). It enables knowledge-based polymorphism assessment based on a statistical analysis of hydrogen bonding patterns. Probabilities for hydrogen bond pairings to form in the target system are calculated from a statistical model built from relevant structures in the CSD. The model encapsulates information regarding the environment of the functional groups, which ensures the prediction is specific to the target molecule. Combining probabilities of hydrogen bond formation with a statistical model that captures information regarding how often a functional group participates allows the generation of chemically sensible alternative structures. The view of the solid state landscape of an active ingredient afforded through the combination of propensity and participation addresses questions such as how likely polymorphism is and whether there is the possibility of a more stable form.

### Integrated data analysis tools

- Sophisticated data analysis tools are now available within Mercury in order to provide statistical, charting and plotting options alongside three-dimensional structural visualization and analysis. This integration enables powerful visualisation and analysis of ConQuest substructure searches where geometric parameters (e.g. bond lengths, angles, torsions etc) have been defined in the query. This functionality replaces that previously provided in Vista. In addition, the new software includes a range of advanced features focused towards structural analysis including principal component analysis, cone-angle correction in hydrogen-bond analyses and the ability to deal with topological symmetry within molecular search fragments.

### Structure solution from powder diffraction data

- The 2012 CSDS release includes DASH at no additional cost for academic subscribers. DASH is a popular and versatile package for solving crystal structures from powder diffraction data and has been used successfully to solve a diverse range of structures including pharmaceutical compounds, salts, solvates, semiconductors and explosives. DASH is also routinely applied to the solution of both organometallic and inorganic crystal structures. The inclusion of DASH as part of the CSDS provides additional benefits including direct links with Mogul for the automatic assessment and use of torsional restraints during structure solution, and the ability to view and compare solutions using the Mercury visualiser.

### **Over half a million unique compounds**

- The 2012 release of the Cambridge Structural Database (CSD v5.33) contains 527,005 unique compounds (refcode families) and a total of 577,833 individual structures including many important polymorphic systems. Throughout 2012 regular data updates will provide access to the latest archived structures. In addition, WebCSD users will gain early access to newly published structures. Flagged as ‘structure pending’ such entries are added to WebCSD on a continual basis as they are published or deposited as Private Communications and evolve into full CSD entries following scientific processing.

## 4. Installation Overview

### 4.1 About This Manual

This manual describes how to install the 2012 release of the Cambridge Structural Database (CSD) System, comprising:

- CSD V5.33
- PreQuest
- ConQuest 1.14
- Mercury 3.0
- Mogul 1.4
- IsoStar 2.1.3

A typical installation will involve the following steps:

- Install the CSD System Software and Database files for Windows (see Section Windows Installation, page 6), Linux (see Section Linux Installation, page 7), and/or for Mac OS X (see Section Mac OS X Installation, page 9).
- Install the IsoStar 2.1.3 server (Linux) (see Section IsoStar 2.1.3 Installation, page 8).
- Register a component of the CSD System software (i.e. ConQuest, Mercury CSD or Mogul) when you first use it (see Section Starting and Configuring CSD System Software, page 12).

### 4.2 System Requirements

#### 4.2.1 Supported Platforms

Executables for ConQuest 1.14, Mercury 3.0, Mogul 1.4, PreQuest and the IsoStar client supplied with this release are supported on the following platforms and operating systems:

- Windows - Intel compatible Windows XP/Vista/7
- Linux - Intel compatible, 32 bit:
  - RedHat Enterprise 4, 5, 6
  - SuSE Linux Enterprise [Desktop|Server] 10, 11
  - Debian 4, 5, 6

*Note:* As we add support for newer versions of Linux, support for older versions may have to be withdrawn.
- Mac Intel compatible:
  - Mac OS X 10.4, 10.5, 10.6, 10.7

The IsoStar server is supported on the following platforms and operating systems:

- Linux - Intel compatible, 32 bit:
  - RedHat Enterprise 4, 5, 6
  - SuSE Linux Enterprise [Desktop|Server] 10, 11
- Debian 4, 5, 6

*Note:* As we add support for newer versions of Linux, support for older versions may have to be withdrawn.

*Note:* the IsoStar server is not supported on Mac OS X or Windows operating systems.

If you choose to use a version other than those listed above we cannot guarantee that CSD System software will work correctly, although we will attempt to assist you with any problems you may encounter.

For more information relating to operating systems and any known problems please see:

[http://www.ccdc.cam.ac.uk/support/supported\\_platforms/platforms.php4](http://www.ccdc.cam.ac.uk/support/supported_platforms/platforms.php4)

#### **4.2.2 Changes to Supported Platforms**

It is anticipated that this release will be the last to support RedHat 4, Debian 4 Linux and MacOSX 10.4 distributions. If this will cause insurmountable difficulties, please contact us at [support@ccdc.cam.ac.uk](mailto:support@ccdc.cam.ac.uk) to discuss possible solutions.

#### **4.2.3 Graphical System Requirements**

The advanced graphical features present in the CSD System software should be compatible with most modern graphical hardware. However, we do highly recommend installation of the latest graphical hardware drivers and OpenGL drivers to ensure optimal performance. These are often both available from your graphical hardware manufacturer's website.

The development and testing of stereo viewing in Mercury 3.0 was done on the following hardware configuration:

- Stereographics CrystalEyes Workstation, with stereo glasses, E2 emitter and StereoEnabler.

Display card:

- NVIDIA Quadro FX 1400.

However, we anticipate that the stereo display should work on any machines that support OpenGL quad-buffered stereo. If you try Mercury 3.0 on machines with any other stereo display, we would appreciate receiving feedback to [support@ccdc.cam.ac.uk](mailto:support@ccdc.cam.ac.uk) on whether this is successful, so that we may inform other users of valid hardware configurations. On machines without appropriate hardware, the **Stereo** check-box will be disabled.

#### 4.2.4 Disk Space Requirements

A complete installation of the Linux version of the 2012 release of CSD System requires approximately 4.6Gb of disk space. This includes ConQuest 1.14, Mogul 1.4, Mercury 3.0, PreQuest, the CSD V5.33 (2.5Gb), and Mogul data files (2.0Gb).

A complete installation of the Windows version of the 2012 release of CSD System requires approximately 4.6Gb of disk space. This includes ConQuest 1.14, Mogul 1.4, Mercury 3.0, PreQuest, the CSD V5.33 (2.5Gb) and Mogul data files (2.0Gb).

A complete installation of the Mac OS X version of the 2012 release of CSD System requires approximately 5.3Gb of disk space. This includes ConQuest 1.14, Mogul 1.4, Mercury 3.0, PreQuest, the CSD V5.33 (2.5Gb), and Mogul data files (2.0Gb).

A complete installation of IsoStar 2.1.3 (including both the data and the software) requires an additional 2.0Gb of disk space.

## 5. Windows Installation

### 5.1 Installation Procedure

The *Windows* DVD-ROM contains ConQuest 1.14, Mercury 3.0, Mogul 1.4, IsoStar PC Client, PreQuest for Windows, CSD database files and Mogul data files for Windows XP/Vista/7

Administrator privileges are recommended but not usually required for installation.

Do not install directly on top of a previous installation; use a new folder. We recommend that you uninstall previous versions of all CSD System software, as well as Mogul and CSD database files, and remove all CSD update files, before you install the current version.

To install on Windows:

1. Load the Windows DVD-ROM:
2. The *CSD SYSTEM SETUP* menu will take you through the steps necessary to install:

CSD System software (ConQuest 1.14, Mercury 3.0, Mogul 1.4, PreQuest for Windows, CSD System database files (the CSD and Mogul data files) and the IsoStar 2.1.3 PC Client

All software and database components are installed via the **Complete CSD System Install** button. We recommend that all default installation paths, as suggested by the installers, are used. If the setup menu does not start automatically then run the following:

X:\maestro\maestro.exe

where X is the drive letter for your DVD-ROM drive.

Alternatively, select *My Computer* and right-click on the appropriate DVD drive and select *Autoplay*.

From the *CSD SYSTEM SETUP* menu select the module you wish to install and follow the on-screen instructions (it is recommended that you run the complete CSD System Installation); you can also browse the release and installation notes.

*Note:* IsoStar 2.1.3 is a client-server application and only the client software can be installed on your Windows PC. A public IsoStar server is now hosted at CCDC: <http://isostar.ccdc.cam.ac.uk>. Access to scatterplots from this public server requires a licensed copy of the IsoStar 2.1.3 client package (see Section Public IsoStar Server, page 23). Alternatively, you can use an HTTP server to make the IsoStar data available. The HTTP server can be run on any of the supported IsoStar Linux platforms (see Section Supported Platforms, page 4). Please note that it is currently not possible to run the server on a PC. More information about how to set-up your HTTP server can be found in (see Section IsoStar 2.1.3 Installation, page 8)

## 5.2 Uninstalling CSD System Software and Database files

The CSD System software can be removed from your computer by selecting:

Start Menu -> CCDC -> CSD System Software 2012 -> Uninstall CSD System 2012

## 5.3 Troubleshooting

If you are running an antivirus program, such as Norton AntiVirus, then you may have problems running ConQuest 1.14 searches and it may be necessary to disable the antivirus software in order to run ConQuest. On startup ConQuest will attempt to identify potential problems with antivirus software when a search is started.

There is some information on the Symantec technical support page, regarding Norton AntiVirus, which allows you to keep an exclusion list to manage exceptions for normal program operations which are being detected as virus-like activities:

Symantec website: <http://www.symantec.com/>

This should allow you to run ConQuest and have Norton AntiVirus running simultaneously.

## 6. Linux Installation

## 6.1 Installation Procedure

The Linux DVD contains the software and databases for Linux.

Do not install directly on top of a previous installation. We recommend that you uninstall previous versions of the CSD system, database files including all CSD update files before you install the current version.

To install the CSD System, and/or data on Linux.

1. Mount the Linux DVD-ROM.
2. As a **non-root** user on the machine you intend to run the CSD System, in a terminal window type:

```
<DVDROM>/csds_2012_linux.run
```

where <DVDROM> is the mount point of your DVD-ROM drive.

Follow the on-screen instructions to install the software and databases.

## 6.2 IsoStar 2.1.3 Installation

The Linux DVD-ROM contains the IsoStar Software for all supported Linux/UNIX platforms, as well as the IsoStar 2.1.3 data files.

To install IsoStar 2.1.3 on Linux:

1. Mount the Linux DVD-ROM.
2. As a **non-root** user on the machine you intend to run the IsoStar server, in a terminal window type:

```
<DVDROM>/Isostar_2012_linux.run
```

where <DVDROM> is the mount point of your DVD-ROM drive.

Follow the on-screen instructions to install the IsoStar server software and databases.

## 6.3 Setting up the CSD System Environment on Linux and Mac OS X

To run PreQuest you must set the CSD environment variable `CSDHOME` and add `CSDHOME/bin`

to your PATH.

1. To set CSDHOME for Bourne shell (sh) or Korn shell (ksh), type:

```
CSDHOME=<CAMBRIDGE>; export CSDHOME
```

where <CAMBRIDGE> is the top level directory of your CSD System installation.

For example:

```
CSDHOME=/usr/local/cambridge; export CSDHOME
```

2. Similarly, to set CSDHOME for C-shell (csh), type:

```
setenv CSDHOME <CAMBRIDGE>
```

where <CAMBRIDGE> is the top level directory of your CSD System installation.

For example:

```
setenv CSDHOME /usr/local/cambridge
```

3. To add CSDHOME/bin to your PATH for Bourne shell (sh) or Korn shell (ksh), type:

```
PATH=$CSDHOME/bin:$PATH; export PATH
```

4. Or for C-shell (csh) type:

```
setenv PATH $CSDHOME/bin:$PATH; rehash
```

To make these changes permanent, add the commands executed in steps 1. and 2. to all your CSD System users' .login (csh) or .profile (sh, ksh) files. Alternatively, place the commands in a system-wide login or profile script such as /etc/profile.

## 7. Mac OS X Installation

### 7.1 Installation Process

The Mac OS X DVD-ROM contains binaries for ConQuest 1.14 for X-Window, Mercury 3.0, Mogul 1.4, IsoStar Client, PreQuest for X-Window, the CSD database files and the Mogul data files. The 2012 CSD System has been prepared on Mac OS X Tiger (10.4) and is also supported on Mac OS X Leopard (10.5), Snow Leopard (10.6) and Lion (10.7). Please use the latest release of Mac OS X.

Administrator privileges are recommended but not usually required for installation.

Do not install directly on top of a previous installation. We recommend that you uninstall previous versions of the CSD system, database files including all CSD update files before you install the current version.

We suggest to install all software and database components in the `/Applications` directory, however you are free to use any other location.

## 7.2 Quick Guide

To install on Mac OS X:

1. Load the Mac OS X DVD-ROM.
2. Double click on `csds_2012_macosx` and follow the on-screen instructions to install the software and databases.

## 7.3 Troubleshooting

Operation of ConQuest, Vista and PreQuest on Mac OS X requires an X server to be running in rootless mode such that X-Window applications can be successfully launched as separate windows on the console display.

IsoStar 2.1.3 is a client-server application and only the client software can be installed on Mac OS X. A public IsoStar server is now hosted at CCDC: <http://isostar.ccdc.cam.ac.uk>. Access to scatterplots from this public server requires a licensed copy of the IsoStar 2.1.3 client package (see Section Public IsoStar Server, page 23). Alternatively, you can use an HTTP server to make the IsoStar data available. The HTTP server can be run on any of the supported IsoStar Linux platforms (see Section Supported Platforms, page 4). Please note that it is currently not possible to run the IsoStar server on Mac OS X. Further information on setting up your HTTP server is provided (see Section IsoStar 2.1.3 Installation, page 8).

Safari does not employ Helper Applications so if this browser is being used to access IsoStar data you will need to download the scatterplot file then open the file within the IsoStar client manually. Alternatively, Firefox can be configured to launch an application associated with a particular file extension.

## 8. WebCSD Access

The 2012 release of the CSD System includes access to WebCSD (the web-based interface to searching the CSD) for those with unlimited site licences. WebCSD can be accessed in two ways:

## **8.1 CCDC Hosted WebCSD Server**

The CCDC hosts a WebCSD server which can be accessed at:

<http://webcsd.ccdc.cam.ac.uk>

Access to this server is restricted by IP address. Those with unlimited site licences can contact [admin@ccdc.cam.ac.uk](mailto:admin@ccdc.cam.ac.uk) with details of their institutions IP address range(s) in order to arrange access.

## **8.2 Locally Installed WebCSD Server**

For industrial users a WebCSD server can also be installed for access at your own site in much the same way as an IsoStar server. Those with unlimited site licences have access to a WebCSD installation DVD that can be used to install this server. For more details please contact [admin@ccdc.cam.ac.uk](mailto:admin@ccdc.cam.ac.uk).

## 9. Starting and Configuring CSD System Software

### 9.1 Windows

To start any CSD system software component on Windows select the appropriate link from the Windows Start menu.

For ConQuest 1.14 select:

Programs -> CCDC -> CSD System Software 2012-> ConQuest

For Mogul 1.4 select:

Programs -> CCDC -> CSD System Software 2012 -> Mogul

For Mercury 3.0 select:

Programs -> CCDC -> CSD System Software 2012 -> Mercury

For IsoStar 2.1.3 client select:

Programs -> CCDC -> CSD System Software 2012 -> IsoStar Client

For PreQuest select:

Programs -> CCDC -> CSD System Software 2012 -> PreQuest

### 9.2 Linux

To start any CSD system software component on Linux, ensure that `$CSDHOME/bin` is in your PATH (see Section Setting up the CSD System Environment on Linux and Mac OS X, page 8).

Then for ConQuest 1.14 (Linux) type:

```
cq
```

For Mogul 1.4 (Linux) type:

```
mogul
```

For Mercury 3.0 (Linux) type:

```
mercury
```

For IsoStar 2.1.3 client (Linux) type:

```
run_isostar
```

For PreQuest type:

prequest

### **9.3 Mac OS X**

To start any CSD system software component on Mac OS X click on the appropriate icon in the Dock, or in the installation folder.

### **9.4 Registration of CSD System Components**

When using any component of the CSD System software (i.e. ConQuest, Mogul or IsoStar client) for the first time you will require your Site Code and Confirmation Code.

**IMPORTANT: confirmation codes for all sites have changed this release. Please refer to the letter accompanying this release for details of your new codes.**

For more information about registration and licensing (see Section CSD System Software Licensing, page 15).

Mercury 3.0 may be installed and used without requiring use of a CSD licence. Licensing Mercury will, however, allow access to additional features that are only available to CSD system subscribers.

## 9.5 Configuration of CSD System Components

### 9.5.1 ConQuest

#### Search Data Directory

Before using ConQuest 1.14 you may be required to identify a Search Data directory. This will be used to store temporary files for running searches. It will also be the default directory for saving some ConQuest files.

#### Database Location

Before using ConQuest 1.14 you may be required to locate the main database files. The location of these files is identified by selecting a CSD database information file. For ConQuest 1.14 this file will be called `as533be.inf` and will be found in the `csd` subdirectory in the location where you installed the database files.

#### Viewing PDF files Produced by ConQuest

ConQuest 1.13 is able to generate PDF files for viewing or printing entries from the CSD (including 2D diagrams).

In order to view or print these files you will need to use Adobe Acrobat Reader. Adobe Acrobat Reader is available from the Adobe web-site: <http://www.adobe.com>.

### 9.5.2 Mogul

#### Database Location

Before using Mogul 1.4 you may be required to locate the main database files (as detailed for ConQuest above) as well as the mogul database files. The location of these files is identified by selecting a mogul path information file. For Mogul 1.4 this file will be called `mogul533.path` and will be found in the `data` subdirectory in the location where you installed the database files.

### 9.5.3 Mercury

When Mercury is launched, it tries to detect whether or not the CSD is installed. If the CSD can be found, it is opened, and the structure navigator on the right hand side of the main Mercury window will then contain the refcodes of all the entries in the database.

If you have a CSD-format database that is not detected automatically by Mercury, you can open it by clicking Databases, followed by Database Location... Once opened the database will be added to the Databases menu.

You can use Mercury to view either your own crystal structures, or those retrieved from a ConQuest search. To view the hits from a ConQuest search in Mercury select Analyse Hitlist, from within ConQuest, and then View in Mercury from the pull-down menu. Alternatively, within ConQuest,

select File from the top-level menu and View in Mercury from the resulting pull-down menu.

Different Mercury features are unlocked depending on your licence (see Section Registering the Different Mercury Components, page 20).

## 10. CSD System Software Licensing

### 10.1 Licensing Overview

As more than one program requires access to the licence information, the licence file is stored in a centralised location, e.g. the directory which contains the main database files. When a product is registered the file *csd\_licence.dat* is created in the CSD database directory or, if this is not possible, either a location will be requested or a *csd\_licence.dat* file will be created in the home directory of the user.

When checking the licence information for a given machine, all the programs will proceed by checking one or more locations for licence data:

- If the environment variable `CCDC_CSD_LICENCE_FILE` is set to a valid filename then this file will be checked.
- The contents of *csd\_licence.redirect* in the database directory will then be examined; any line not starting with # will be checked to see if it is the name of a valid licence file that can be accessed. If any can be accessed then these will be checked and the first one possible used.
- The file *csd\_licence.dat* in the main database directory will then be checked.
- In the unlikely event that it is not possible to write to any of the possible licence file locations, some programs (Mogul or Mercury) may allow you to save and/or locate the licence data in a different location to the above. If this has been done, this location will be checked.
- If a *.csd\_licence.dat* is located in the home directory of the user (`/home/user` on Linux / `documents and settings/user` on WindowsXP, `/users/user` on Windows Vista/7), this will be checked last.

If a valid licence for the machine cannot be located, the machine will have to be licensed i.e. a component of the CSD System software will have to be registered on the machine (see Section Registration Overview, page 16).

The file *csd\_licence.redirect* can be used in the event that the directory containing the database files is read-only, meaning it is not possible to write any licence information to the *csd\_licence.dat* file. In this case, the filename(s) of one or more licence files (found in writable locations) should be added to the *csd\_licence.redirect* file; these files can then be used instead of the *csd\_licence.dat* file. Note that it is possible to include both Windows and Linux filenames in this file.

If any of the *csd\_licence.redirect* and *csd\_licence.dat* approaches do not work, the

CCDC\_CSD\_LICENCE\_FILE environment variable can be set to point all the applications to a different location. For example, to use a similar method to previous releases you could set CCDC\_CSD\_LICENCE\_FILE to <conquest\_dir>/csd\_licence.dat.

This licensing system is particularly suitable for users with unlimited licences who can then take advantage of the IP licensing option (see Section IP-Based Licensing, page 20).

## 10.2 Registration Overview

CSD System software is licenced on a node-locked basis. Your site has a Licence of Access Agreement that entitles you to install the CSD System on a specified number of machines.

The first time you attempt to run any of the CSD System components (i.e. ConQuest 1.14, Mercury 3.0, Mogul 1.4) on a particular machine you will be prompted to register the installation using the process described below.

*Note:* For those institutions with a site licence an IP-based licencing mechanism is available. This mechanism provides site-wide access to the CSD without the need to register individual machines (see Section IP-Based Licensing, page 20).

CSD System software registrations are machine specific. You must register a single CSD System component (i.e. ConQuest, Mogul, IsoStar client or Mercury CSD) separately on each machine on which it is to be used. This results in a different Validation Number for each machine.

1. If you already have a current CSDS licence, hit the **Locate file containing valid licence** button (see Section Specifying an Existing Licence File, page 17).
2. Enter your Site Code and 6-digit Confirmation Code in the dialogue box shown below (the registration window shown is for ConQuest, however a similar window will appear if using Mogul or Mercury for the first time). These codes are supplied in a letter accompanying this release.

**IMPORTANT: confirmation codes for all sites have changed with the 2012 release. Please ensure you use your updated codes when registering.** (In some circumstances the Codes will already be displayed in the dialogue box):



3. Attempt to register online by hitting the **Register Online** button in the dialog box (see Section Online Registration, page 17).
4. If your machine is not connected to the internet or if online registration fails you must register offline (see Section Offline Registration, page 18).

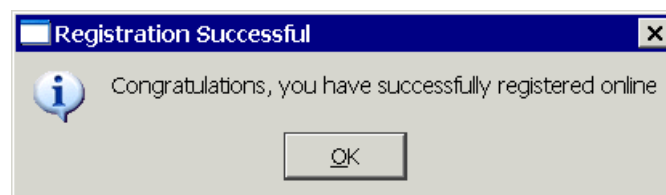
### 10.3 Specifying an Existing Licence File

If you already have an existing *csd\_licence.dat* file, hit the **Locate file containing valid licence** button at the top of the *CCDC Product Registration* dialogue. From within the resultant Specify licence file location window, browse to the directory containing the licence file, select the *csd\_licence.dat* file then hit the **Open** button.

### 10.4 Online Registration

To register online, hit the **Register Online** button.

If online registration is successful you will see the following dialogue box:



*Note:* When registering ConQuest, Mogul, or Mercury in this way it is possible to purchase additional licences online by clicking on the **Buy Additional Licences Online** button in the corresponding *Online Registration* window.

If the number of machines on which CSD System Software has been run at your site exceeds the number specified in your Licence of Access agreement then you will be offered some or all of the following options:

- Register CSD System software on this machine as an evaluation.

*This option is only available online.*

- Purchase an additional CSD System software licence.

*Valid provided that your basic CSD subscription does not lapse. In order to purchase additional CSD System software licences you must contact the CCDC using the phone, fax or email address displayed, or use the online service.*

- Transfer an existing CSD System software licence from another machine.

*This option is available online and enables you to reassign one of your existing CSD System software licences from another machine. This may be necessary if, for example, the original machine has been decommissioned or has suffered a system crash. The number of times that licences can be reassigned is limited so this option may not be available. If you wish to transfer a licence but you are not offered this option then please contact the CCDC using the phone, fax or email address displayed.*

## **10.5 Offline Registration**

If your machine is not connected to the internet or if online registration fails you must register offline. In order to do this you will need to send the following information to the CCDC by email:

- Site Code
- Confirmation Code
- Serial Number

The Serial Number will be displayed in an extension to the original Registration dialogue box which appears after you hit the **Register Offline** button:

Locate file containing valid licence or register below.

**You must register to be able to use ConQuest. This registration will also allow you to use certain other CSD Products.**

Please enter your site number and confirmation code (found on your accompanying letter) and select the **'Register Online'** button.

If you are unable to register online please select **'Register Offline'** to activate the offline registration section.

For more information licencing select the **'Help'** button.

Site Number: 1234      Confirm Code: 123456      Buy Additional Licences Online

Register Online   Register Offline   Help   Abort

To **Register Offline**, please contact CCDC with the following information:

No: 1111, Confirm Code: 123456, Serial No: 9033-a112-2f34-1e15

Automated Email: *licence@ccdc.cam.ac.uk*  
 Other Licence Enquiries: *licence\_help@ccdc.cam.ac.uk*  
 Fax: +44 1223 336033 Phone: +44 1223 336394

After your information has been checked you will be given a **validation code**. This code should be entered below either now or next time you try to start this program.

Note that copy/paste of the validation code into any of the boxes below should work.

-  -  -  -   
 -  -  -       Register

The Site Code, Confirmation Code and Serial Number can be copied and pasted from the Registration dialogue box and sent by email to: *licence@ccdc.cam.ac.uk*

You should automatically receive a Validation Number by return email.

To complete your registration you must enter this Validation Number in the space provided at the bottom of the Registration dialogue box as it appears after the **Register Offline** button has been hit.

If you are unable to obtain a Validation Number by automated email then contact the CCDC with your Site Code, Confirmation Code and Serial Number using:

Email: *licence\_help@ccdc.cam.ac.uk*  
 Phone: +44 1223 336394

and a Validation Number will be issued to you.

## 10.6 Registering the Different Mercury Components

Accessing CSDS features:

- If Mercury 3.0 is started before ConQuest 1.14 or Mogul 1.4 are registered, only a base level version of Mercury will be available. A small CCDC icon will be shown against all the menu items and main-window widgets that are unavailable in this version. You will need to register Mercury to access CSDS features. Registration can be done in one of three ways:
  - Mercury will prompt you for a site code and confirm code when it is first started, if ConQuest or Mogul has not already been registered.
  - A pop-up will appear if any of the registered features are selected. Follow the on-screen instructions.
  - Go to **Help, Register Mercury** and follow the instructions.

Accessing the Solid Form module:

- The Solid Form module of Mercury is usually available at no additional cost to academic Cambridge Structural Database System subscribers. Industrial customers should contact *admin@ccdc.cam.ac.uk* for further information. Evaluations are normally available for those industrial organisations interested in purchasing.
- Licensing of the Solid Form module of Mercury is handled through the existing CSD licensing system and the *csds\_licence.dat* file. To register the Solid Form module in a copy of Mercury CSD where it is currently not activated, select the **Register Solid Forms module...** option from the *Help* menu. Registration can be completed both online and offline as described above for the CSD System.

The **Help, About Mercury...** menu option will display details about your current licensing status, including the Solid Form module.

## 10.7 IP-Based Licensing

An IP-based licensing mechanism is available to institutions with site licences. This mechanism enables site-wide access to the CSD without the registration of individual machines.

The licensee should nominate a number of individual IP addresses, or ranges, which are authorized to access the CSD System. IP addresses should be provided in an email and sent to:

*licence\_help@ccdc.cam.ac.uk*

The addresses provided will then be encrypted into a licence key (*csd\_licence.dat*) that will allow ConQuest to operate on those machines. The *csd\_licence.dat* file can either be distributed from a central location or copied to each local client installation. The *csd\_licence.dat* file should be copied to the following central locations:

**Linux:**

```
$CSDHOME/csd/csd_licence.dat
```

**Windows:**

```
<InstallDIR>\CSD V533\csd_licence.dat  
where <InstallDIR> is, e.g., C:\Program Files\CCDC
```

The licensing system is particularly suitable for use with IP licensing. We will be able to provide you with IP licence data that can be stored in the central *csd\_licence.dat*. The whole directory can then be set as read only for safety and every program will be able to retrieve and use the licence data.

**10.8 Registration Problems**

Under some circumstances ConQuest may have problems saving the registration information. This is most likely to happen when the ConQuest files are located on a different machine and mounted in such a way that the machine being registered is not able to write to the central validation file: (<CAMBRIDGE>/csd/csd\_licence.dat).

If this happens ConQuest will produce a pop-up listing the Serial Number and the Validation Number for that machine. The following action should be taken in order to complete the registration procedure on this machine.

Either:

- Log into a user account on a machine which does have write access to the validation file and register ConQuest as that user.

Or:

- On a different machine that can write to the validation file, edit *csd\_licence.dat* and add a line similar to the one shown below. You will need to make sure that the hyphens in the serial numbers are represented as underscores:

```
SN_1111_2222_3333_4444 = ('hostname', '1111-2222-3333-4444-5555-6666-7777-8888-9999')
```

Where the digits after *SN\_* are the Serial Number given in the pop-up, *hostname* is the name of the machine and the final set of digits are the Validation Number given in the pop-up.

*Note:* the nine blocks of four characters above are for Windows, Linux and Mac OS X operating systems; on UNIX there will be five blocks of four characters.

We are aware that some sites may have difficulty registering online due to the use of a local proxy server. In such cases it is necessary to set the proxy server information via the **proxy** button on the CCDC product registration dialog prior to clicking on **Register Online**.

## 10.9 Current Licence Information

It is possible to look at your current licence usage and allowances, and to purchase additional licences for ConQuest, Mogul and Mercury online:

*[http://www.ccdc.cam.ac.uk/products/csd\\_system/conquest/purchase\\_licences/](http://www.ccdc.cam.ac.uk/products/csd_system/conquest/purchase_licences/)*

*Note:* you will need to enter your Site Number and Confirmation Code on this page in order to proceed. It is also possible to gain access to this licensing information page from within ConQuest by selecting **Help** in the top-level menu and then selecting **Current Licence Information** from the resulting pull-down menu. Additional licences can be purchased by clicking on **Help** in the top-level menu and then selecting **Purchase Extra Licences** from the resulting pull-down menu.

The resultant page is divided into 3 sections:

- Basic site information
- Licence summary and any details of individual licences used, such as serial number, validation code, registration method (including IP-address if registered online) and time of registration
- Online purchasing of additional ConQuest Licences (more information on this is given below)

## 10.10 Online Licence Purchasing

The online purchasing section will normally contain a pull-down list of options from which you can select the number of additional licences you wish to purchase. This facility is not available to certain sites, who should continue to use their current method for payment of licence fees. A notice will be displayed indicating that this applies to your site.

Once you have selected the number of additional licences that you wish to purchase, select the **Proceed with Purchase** button which will transfer you to the WorldPay secure server. Here you will be able to enter your credit card details. At the end of the transaction you will be transferred back to the CCDC website and confirmation of any additional licences purchased will be displayed; these licences are available for immediate use. An email confirmation will be sent.

*Note:* European Community customers, for whom the CCDC does not hold a valid VAT number, will be prompted to enter the VAT number of their organisation before proceeding with any purchase. If no VAT number is entered at the prompt the resultant prices will include VAT.

Where a site has already purchased additional licences (either online or offline) the price of a site licence will be adjusted accordingly to take into account the payment already made.

## 11. Public IsoStar Server

A public IsoStar server is now hosted at CCDC: <http://isostar.ccdc.cam.ac.uk>. Access to scatterplots from this public server requires a licensed copy of the IsoStar 2.1.3 client package.

## 12. CSD Data Updates

It is possible to download CSD data updates which are produced at regular intervals (approximately every 3 months). This will keep your copy of the CSD more current between each major release of the CSD System.

Data updates can be obtained automatically via the **Help... Check For Updates** option in Mercury.

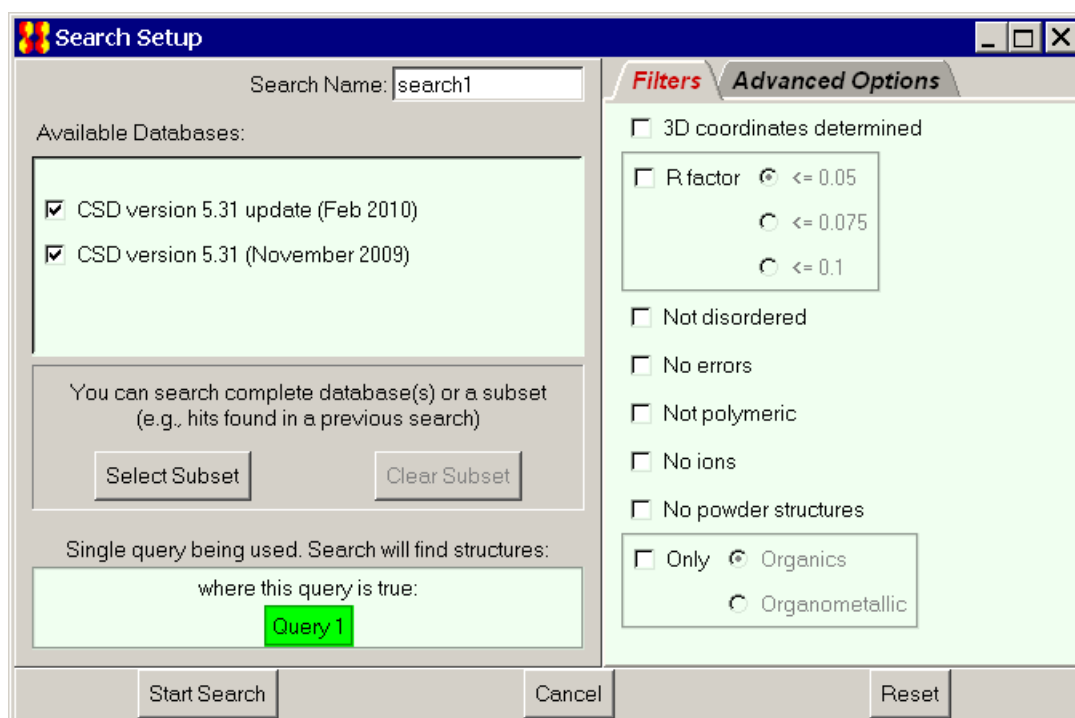
Alternatively, the following URL will take you to the download page which describes what you need to do to obtain the updates manually:

[http://www.ccdc.cam.ac.uk/products/csd\\_system/conquest/csd\\_updates/](http://www.ccdc.cam.ac.uk/products/csd_system/conquest/csd_updates/)

- You will be required to enter your Site Code and Confirmation Code in order to download an update.
- The updates will need to be downloaded in numeric order and added to the same directory as your CSD database files.
- Follow the instructions for installation and the update(s) will be visible when restarting ConQuest.

*Note:* You will need write permission to the main CSD folder to install each update.

- Each update will be shown separately in the *View Databases* menu.
- The update packages can be searched either with the main database or separately as desired; this is controlled via options in the *Search Setup* dialogue box:



### 13. Activating In-House Databases

ConQuest 1.14 can search in-house databases in addition to the main CSD. These databases are created using the PreQuest program. If you have created an inhouse database that you wish to search using ConQuest you must first activate it using the procedure described below.

In order to activate your in-house database you must copy (or soft-link: Linux only) the three in-house database files (*.ind*, *.msk* and *.tcd*) to the same directory as the CSD V5.33 database files. On Linux/UNIX this is typically:

```
<CAMBRIDGE>/csd
```

While on PC, this is normally:

```
C:\Program Files\CCDC\CSD V533
```

You must then run the Activate program.

For Linux, ensure that `$CSDHOME/bin` is in your `PATH` (see Section Setting up the CSD System Environment on Linux and Mac OS X, page 8) and type:

```
activate
```

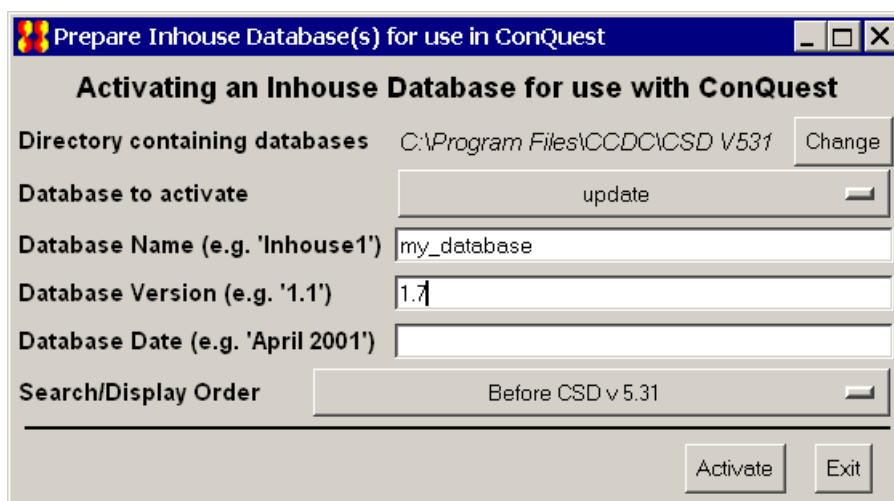
To run the *activate database* program on a PC select:

```
Programs -> CCDC -> CSD System Software 2012-> Activate in-house database
```

from the Windows Start menu.

*Note:* Windows Vista/7 users will require escalated administrator privileges to activate databases. To do so, right-click on the **Activate Inhouse Databases** menu item and select **Run as Administrator**.

In both cases a pop-up window like the one shown below will be displayed:



The activation program attempts to find the directory where the database is located by examining your ConQuest defaults file. However, if the correct directory cannot be found then use the **Change** button to locate the required directory.

All databases in the selected directory which have *not* been activated will be displayed in the **Database to activate** pull-down menu. Simply select the databases you wish to activate.

The contents of the **Database Name** dialogue box will be used by ConQuest to identify which databases you wish to search or view. Choose a name relevant to the database contents.

Enter a version number for the database in the **Database Version** dialogue box. If you have an earlier version of a database, with the same Database Name in the same directory, it is important to make sure that the most recent version has the largest version number so that it is used in preference to the others.

Enter the date for the database in the **Database Date** dialogue box.

Use **Search/Display Order** pull-down menu to select the order in which activated databases will be displayed and searched by ConQuest. Taking the above example, if you select **After CSD v5.33**, when both databases are selected for searching in ConQuest the main CSD database will be searched before the in-house database.

When you are happy with your selections press the **Activate** button. This will create a `.inf` file for the database, which will then be viewable and searchable the next time you start ConQuest. You can activate additional databases by repeating the procedure described above.

To close the *activate database* program press the **Exit** button.

## 14. Classroom ConQuest

Classroom ConQuest is a version of ConQuest which has been designed for group teaching activities.

- Anyone with at least one normal ConQuest licence can install as many copies of Classroom ConQuest as they require.
- It has all the functionality of *normal* ConQuest with the limitation that searches can only be done on a subset of entries.
- The subset of entries can either be the default selection supplied with Classroom ConQuest or one derived by the user from the main CSD.

*Note:* Classroom ConQuest licences do not allow access to Mogul or additional functionality in Mercury.

### 14.1 Installing Classroom ConQuest

It is possible to register ConQuest 1.14 as a Classroom version. In order to install Classroom ConQuest you must first obtain a Classroom ConQuest Validation Number from the CCDC.

To obtain a Classroom ConQuest Validation Number please contact the CCDC with your Site Code and Confirmation Code using:

Email: [licence\\_help@ccdc.cam.ac.uk](mailto:licence_help@ccdc.cam.ac.uk)

Phone: +44 1223 336394

and a Classroom ConQuest Validation Number will be issued to you.

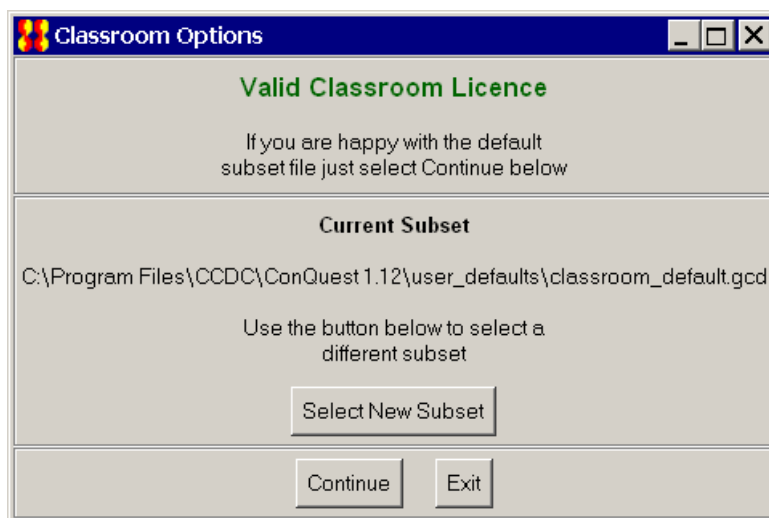
Once you have obtained your Classroom ConQuest Validation Number proceed as for a *normal* ConQuest installation up to the point of registration. At registration select **Register Offline** and enter your Classroom ConQuest Validation Number in the boxes at the bottom of the dialogue box. Provided that the number that you have entered is valid the following pop-up will appear:



- If you select **no** then the Validation Number will be linked only to the machine on which you are registering Classroom ConQuest. This is similar to standard registration procedure.
- If you select **yes** then ConQuest will run on any machine that shares the same Validation file as the machine on which you registered. Selecting yes can be useful when you wish to install Classroom ConQuest on a cluster of machines as in this case you need only enter the Classroom ConQuest Validation Number once. This will not affect versions of ConQuest that have been registered in the normal way.

## 14.2 Basics of Using Classroom ConQuest

Each time a *classroom registered* version of ConQuest is started it will produce a dialogue box similar to the following:

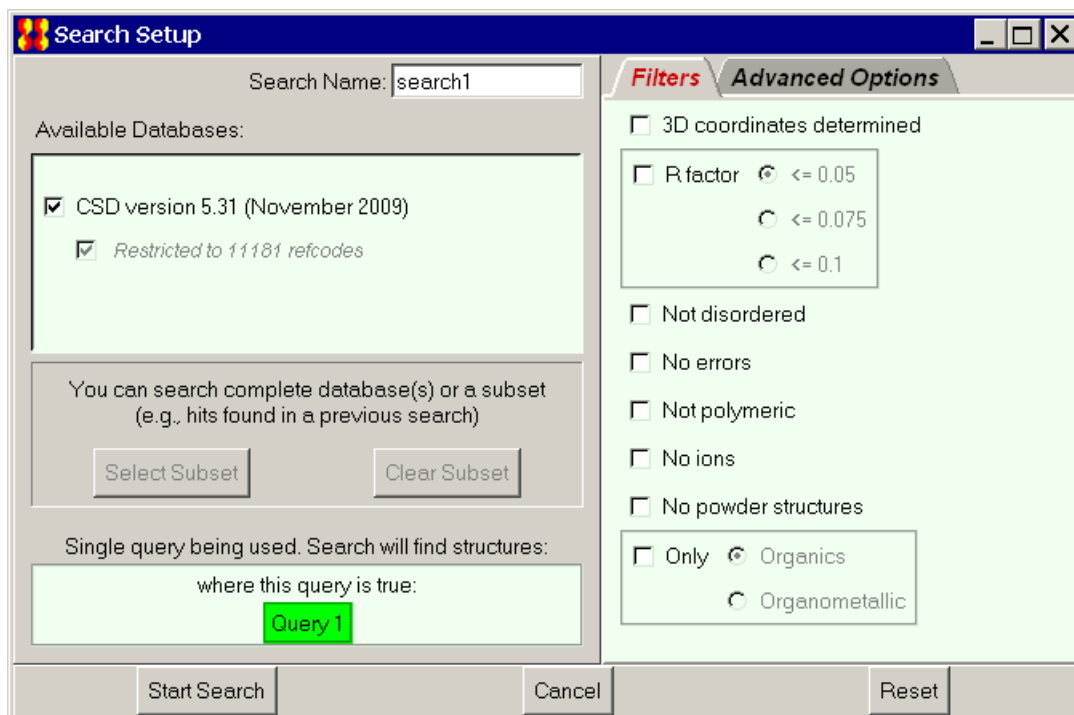


The aim of this dialogue box is to:

- Tell you if the Classroom licence has expired.
- Allow the selection of a different subset for the duration of the session (see Section Choosing a Subset, page 28).

Within ConQuest everything is normal except for the *Search Setup* dialogue box, which indicates that:

- Only the main CSD is available.
- Searches are restricted to a subset of refcodes (the associated check-button is disabled so that it cannot be changed).
- The **Set Subset** and **Clear Subset** buttons are inactive.



### 14.3 Choosing a Subset

The subset used by Classroom ConQuest is specified by a file containing a list of CSD refcodes.

The default refcode list is `classroom_default.gcd` which is located in the `user_defaults` directory.

You can elect to use a different subset of up to one fifth of the number of entries in the current version of the CSD. This can be done by:

- Replacing the default file with a new one that has the same name.
- Editing `user_defaults/conquest_options` so that the line beginning `classroom_refcode_list = ...` indicates the location of the refcode list to be used (specify the full path). For Windows use forward slashes (/) in the path instead of back slashes (\).
- Selecting a different subset using the **Select New Subset** button to select a different refcode list.

This button is displayed when each Classroom ConQuest session is started (see Section Basics of Using Classroom ConQuest, page 27).

Although Classroom ConQuest will start if your refcode list is too big, it will issue an error message when you attempt to start a search.

