CSD Release and Installation Notes

2017 CSD Release

Conditions of Use

The Cambridge Structural Database System (CSD System) comprising all or some of the following: ConQuest, Quest, PreQuest, deCIFer, Mercury, (Mercury CSD and CSD-Materials [formerly known as the Solid Form or Materials module of Mercury], Mercury DASH), Mogul, IsoStar, DASH, SuperStar, web accessible CSD tools and services, WebCSD, CSD Java sketcher, CSD data file, CSD-UNITY, CSD-MDL, CSD-SDFile, CSD data updates, sub files derived from the foregoing data files, documentation and command procedures, test versions of any existing or new program, code, tool, data files, sub-files, documentation or command procedures which may be available from time to time (each individually a Component) is a database and copyright work belonging to the Cambridge Crystallographic Data Centre (CCDC) and its licensors and all rights are protected. Use of the CSD System is permitted solely in accordance with a valid Licence of Access Agreement or Products Licence and Support Agreement and all Components included are proprietary. When a Component is supplied independently of the CSD System its use is subject to the conditions of the separate licence. All persons accessing the CSD System or its Components should make themselves aware of the conditions contained in the Licence of Access Agreement or Products Licence and Support Agreement or the relevant licence.

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Cambridge Crystallographic Data Centre
12 Union Road
Cambridge CB2 1EZ, United Kingdom

Web: http://www.ccdc.cam.ac.uk
Telephone: +44-1223-336408
Email: admin@ccdc.cam.ac.uk

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Contents

1   CSD Release Package

The 2017 CSDS installer is supplied via download, or via USB stick, for Windows, Linux (32-bit and 64-bit) and Mac OS X. The 2017 CSDS installer contains these components:

- The Cambridge Structural Database, Version 5.38
- ConQuest 1.19
- Mercury 3.9
- enCIFer 1.5.2
- IsoStar 2.2.4 (Server is Linux 32-bit only)
- Mogul 1.7.2
- PreQuest (Windows and Linux 32-bit only)
- Conformer Generator 1.1
- Hermes 1.8.2
- GOLD 5.5
- SuperStar 2.1.4 (Windows and Linux only)
- DASH 3.3.6 (Windows only)
- CSD Python API 1.3 (not supported on Windows XP)

Supported platforms are listed elsewhere (see Supported Platforms).

Additionally, you may have access to other components that are supplied separately:

- WebCSD (accessed via webcsd.ccdc.cam.ac.uk)
- Relibase (provided separately via a USB disk)

Access to these will depend on what your licence gives you access to:

CSD-System

- ConQuest, Mercury, PreQuest, Mogul, IsoStar, WebCSD, enCIFer and the CSD Python API.

CSD-Materials

Everything in CSD-System as well as:

- Additional functionality within Mercury and the CSD Python API.
- Conformer Generator and DASH.

CSD-Discovery

Everything in CSD-System as well as:

- Additional functionality within Mercury and the CSD Python API.
- Hermes, GOLD, SuperStar, Relibase and Conformer Generator

CSD-Enterprise

All of the above

2 Database Content and Information

- The number of CSD entries in the 2017 release of the CSD System is 843,799 in the main database and 14,856 in the Nov16 update, making a total of 858,655.

3   What's New

The CSD Database

- The 2017 release contains over 840,000 entries (CSD version 5.38) – an increase of more than 55,000 entries
- Targeted enhancements have also been made to a record-breaking 73,985 existing CSD entries, including:
    - Enrichment of pharmaceutical structures, including addition of DrugBank IDs
    - Addition of validated metal oxidation states to over 21,000 entries
    - Inclusion of article DOIs for many older entries
    - Manual addition of structures from non-electronic data
    - Enhancement of many entries from 35 years of historical structures

CSD-System

- The new CSD Python API has been improved for usability include:
    - Seamless installation of the CSD Python API within the CSD 2017 release
    - An upgraded CSD Python API menu in Mercury with even more scripts
- Enhancements to Mercury and ConQuest including the ability to:
    - Make use of touch-screens with Mercury for pinch, pan and zoom
    - Sketch a molecule within Mercury and convert to a 3D model
    - Perform additional crystallographic transformations in Mercury (such as inversion, switching space group settings or changing origin choice)
    - Utilise two new metal-organic framework (MOF) subsets within ConQuest

CSD-Materials

- Enhancements have been made to the graphical user interface for studying crystal packing similarity and dissimilarity
- Significant advances have also been made in the layout and usability of the Hydrogen Bond Propensity application
- The quality of conformers containing flexible rings produced using our CSD-driven Conformer Generator has been improved

CSD-Discovery

- Improvements have been made in our leading docking software GOLD including the ability to:
    - Make the most of your unlimited processes with streamlined licensing on clusters
    - Automate and integrate preferred workflows with our first implementation of GOLD in the CSD Python API
    - Receive faster more robust development of GOLD in the future as a result of extensive updates to the underlying code
- CSD-Discovery now includes a complete ligand-based workflow allowing you to:
    - Produce experimentally realistic ensembles of conformers using our CSD-driven Conformer Generator
    - Generate your pharmacophore from known binders using the improved Ligand Overlay application
    - Screen your virtual library using the Field-Based Ligand Screener in the CSD Python API Python

4   Known Problems

- **Unattended Installation:**
  If installing the CSDS software via unattended command line mode to a location that already contains a previous installation of the CSDS software, then installation of the CSD Python API will fail. Please ensure you install to a directory without CSD_2017, GoldSuite_2017 or Python_API_2017 subdirectories.

- **Registering via ConQuest on MacOS 10.12:**
  Registering on MacOS 10.12 can cause ConQuest to give an uncaught exception error. This does not affect the registration process and can be safely ignored. Registration by any other means should not cause the error to appear.

- **Use of the 'Locate Licence File' option to specify a licence file:**
  This functionality will only allow you to use a licence file in a non-standard location for the session you are using the CSD software for. In order to have a licence permanently used, please use one of the methods detailed in CSD System Software Licensing.

- **Use of Matplotlib and Pillow in the included CSD Python API miniconda**:

  The versions of matplotlib (1.4.3) and Pillow (2.8.2) that we bundle with our miniconda distribution can cause crashes to occur if used in interactive mode. A workaround for the problem is to replace "matplotlib.show()" with

  "matplotlib.show(block=False)"

- **PreQuest is not compatible with Ubuntu 14 and 16:**
  PreQuest will fail to launch on Ubuntu 14 and 16. We would recommend using one of the other supported platforms to enable use of PreQuest.

- **IsoGen**:

  If you use IsoGen to generate your own IsoStar scatterplots please use ConQuest 3D constraints between groups rather than atoms when you perform the initial ConQuest search, otherwise you will not be able to generate contours for the plots. Please see the IsoGen guide in the IsoStar documentation for further details.

- **Use of ConQuest's 3D Visualiser on Retina Displays:**
  On Mac OSX systems with retina displays only, there is a known issue with being unable to select atoms in ConQuest's 3D visualiser. We would recommend exporting your hits to Mercury for further analysis instead.

5   Installation Overview

This section describes how to install the 2017 release of the Cambridge Structural Database (CSD) System, comprising:

A typical installation will involve the following steps:

1. Download the required CSD System installers from http://www.ccdc.cam.ac.uk/csds_download. This will require your Site Number and Confirmation Code.

2. Install the CSD System Software and Database files for Windows (see Windows Installation), Linux (see Linux Installation), and/or for Mac OS X (see Mac OS X Installation) and registering the software.

3. Install the IsoStar 2.2.4 server (Linux) (see IsoStar 2.2.4 Installation).

5.2   System Requirements

5.2.1   Supported Platforms

Executables in this release are supported on the following platforms and operating systems, unless noted that some platforms are unavailable in section 1:

- Windows - Intel compatible, 32-bit executables (compatible with 32-bit and 64-bit versions of Windows) for:
    - Windows XP*, Vista, 7, 8 and 10
- Linux - Intel compatible. Both 32-bit and 64-bit versions are available for:
    - RedHat Enterprise 6 and 7
    - CentOS 6 and 7
    - Ubuntu 12, 14 and 16
      Note: As we add support for newer versions of Linux, support for older versions may have to be withdrawn.
- Mac Intel compatible 64-bit executables for:
    - Mac OS X 10.9, 10.10, 10.11 and 10.12

* The CSD Python API is not supported on Windows XP

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.

5.2.2   Changes to Supported Platforms

This release adds support for Ubuntu Linux 16, MacOS 10.12.

This release no longer supports SuSe Linux and RedHat/CentOS 5 or Mac OS X 10.8.

It is anticipated that this release will be the last to support Windows XP and Vista, as well as Mac OS X 10.9.

Note that withdrawal of support does not necessarily mean that our future software releases will not work on that platform, but that we cannot guarantee we will be able to do so as software will not be fully tested on those systems. If this will cause insurmountable difficulties, please contact us at *support@ccdc.cam.ac.uk* to discuss possible solutions.

5.2.3   Stereoscopic Viewing Graphical System Requirements

Please check the following support solution on our website to see the most recent recommendations for 3D stereoscopic viewing in Mercury:

http://www.ccdc.cam.ac.uk/SupportandResources/Support/pages/ SupportSolution.aspx?supportsolutionid=284

We would appreciate receiving feedback to *support@ccdc.cam.ac.uk* on your experiences of using stereo display on different hardware configurations to those suggested in the support solution above, if successful, so that we may inform other users of valid hardware configurations. On machines without appropriate hardware, the **Stereo** check-box will be disabled.

5.2.4   Disk Space Requirements

A complete installation of the 2017 release of CSD System requires approximately 17 Gb of disk space. This includes all software (3 Gb) and all data files (14 Gb).

6   Windows Installation

6.1   General Installation Options

On all platforms the installer will give you the option to install:

- CSD Software
- CSD Data

The default option is to install both the CSD Software and the CSD Data to the same location. However, it is possible to install the CSD Software and CSD Data separately. In this case we recommend installing the CSD Data to your desired location first, then re-run the installer and install only the CSD Software - you will be prompted to locate the CSD Data so that individual users will not need to do so themselves when first starting CSD software that requires it.

6.2   Installation Procedure

Administrator privileges are recommended 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, any previous version of the CSD Python API, 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. Download the csds-2017-windows.zip file and unpack its contents to a location on your computer. Note that the installer cannot be run from within the zip file and both the installer and dist file must be located in the same directory.

2. Double-click on the csds-windows.exe file. The installer menu will take you through the steps necessary to complete the installation.

3. Installation will place ConQuest, Mercury, Mogul, Conformer Generator and IsoStar Client in a 'CSD_2017' sub-directory, and Hermes, GOLD and SuperStar in a 'GoldSuite_2017' sub-directory, and the CSD Python API in a 'Python_API_2017' sub-directory. Shortcuts to these programs will also be placed on your desktop and Start Menu (where available).

6.3   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 2017 -> Uninstall CSD System 2017

7   Linux Installation

7.1   Installation Procedure

Linux versions of the CSD software are provided for both 32- and 64-bit versions of linux. Please ensure that you download the correct version for your version of 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. Download csds-2017-linux.tar (32-bit) or csds-2017-linux-x64.tar (64-bit) and unpack its contents to a location on your computer. Note that both the installer and dist file must be located in the same directory.

2. Ensure that the installer executable has execute permissions via the command:

    ```
    chmod a+x ./csds-linux.run
    ```

    if installing the 32-bit version, or

    ```
    chmod a+x ./csds-linux-x64.run
    ```

    if installing the 64-bit version.

3. As a **non-root** user on the machine you intend to run the CSD System, in a terminal window type:

    ```
    ./csds-linux.run
    ```

    or

    ```
    ./csds-linux-x64.run
    ```

    Dependent on the version you unpacked in the previous steps.

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

7.2   IsoStar 2.2.4 Server Installation

This step may be skipped entirely if you wish to use our publically hosted IsoStar server at http://isostar.ccdc.cam.ac.uk.

The Linux IsoStar Server installer contains the IsoStar Software for all supported Linux 32-bit platforms, as well as the IsoStar 2.2.4 data files.

To install IsoStar 2.2.4 on Linux:

1. Download the IsoStar-2.2.4-linux-installer.run installer file.

2. Ensure that the installer executable has execute permissions via the command:

    ```
    chmod a+x ./IsoStar-2.2.4-linux-installer.run
    ```

3. As a **non-root** user on the machine you intend to run the CSD System, in a terminal window type:
    ```
    ./IsoStar-2.2.4-linux-installer.run
    ```

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

8   Mac OS X Installation

8.1   General Installation Process

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, which will usually require Administrator privileges. However, you are free to use any other location.

8.2   Installation Procedure

To install on Mac OS X:

1. Download the csds-2017-osx.tar file and unpack its contents to a location on your computer. Note that both the installer and dist file must be located in the same directory.

2. Double click on `csds-osx` and follow the on-screen instructions to install the software and databases.

8.3   Troubleshooting

Operation of ConQuest 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. A suitable X11 server can be downloaded from *http://xquartz.macosforge.org*.

IsoStar 2.2.4 is a client-server application and only the client software can be installed on Windows or Mac OS X. A public IsoStar server is hosted at CCDC: *http://isostar.ccdc.cam.ac.uk*. Access to scatterplots from this public server requires a licensed copy of the IsoStar 2.2.4 client package (see Public IsoStar Server). 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 Supported Platforms). Please note that it is currently not possible to run the IsoStar server on Windows or Mac OS X. Further information on setting up your HTTP server is provided (see IsoStar 2.2.4 Installation).

On Mac OS X, 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.

If you are experiencing any problems with installation or use of the CSD System, please review our support database at *http://www.ccdc.cam.ac.uk/support* where you should be able to find help with common issues.

9   WebCSD Access

The 2017 release of the CSD System includes access to WebCSD (the web-based interface to searching the CSD). WebCSD can be accessed in two ways:

9.1   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 or if you are a member of an academic institution you will be able to register a username and password in order to obtain access. When your academic institution has purchased a campus licence you will receive unlimited, site-wide access to WebCSD.

Those with unlimited site licenses can contact admin@ccdc.cam.ac.uk with details of their institutions IP address range(s) in order to arrange access.

9.2   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 licenses have access to a WebCSD installer that can be used to install this server. Alternatively, we can arrange to send industrial users ISOs for additional ease of accessibility. For more details please contact *admin@ccdc.cam.ac.uk*.

10   Starting and Configuring CSD System Software

10.1   Windows

To start any CSD system software component on Windows select the appropriate link from the Windows Start menu (Windows XP/Vista/7):

>   Programs -> CCDC -> CSD System Software 2017

Or use one of the desktop shortcuts created for ConQuest, Mogul, Mercury, IsoStar, enCIFer, DASH, Hermes and GOLD by the installation process.

10.2   Linux

Using a command line console, change directory to <INSTALLDIR>/CSD_2017/bin (where <INSTALLDIR> is the path to your CSD_2017 installation directory), or ensure that this is in your system PATH.

Then for ConQuest, type:

```
cq
```

For Mogul, type:

```
mogul
```

For Mercury, type:

```
mercury
```

For IsoStar client, type:

```
run_isostar
```

For PreQuest, type:

```
prequest
```

For GoldSuite software, change directory to <INSTALLDIR>/GoldSuite_2017/bin (where <INSTALLDIR> is the path to your GoldSuite_2017 installation directory), or ensure that this is in your system PATH.

Then for Hermes, type:

```
hermes
```

For the GOLD interface in Hermes, type:

```
gold
```

10.3   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 for ConQuest, Mercury, Mogul, IsoStar, enCIFer, Hermes and GOLD.

10.4 Using Hermes to access GOLD, SuperStar and Relibase+ functionality

Hermes acts as both a visualiser and as an interface and client for GOLD, SuperStar and Relibase+ functionality. Access to these requires a CSD-Discovery enabled licence.

SuperStar can be accessed via the Calculate menu and GOLD can be accessed via the GOLD menu.

Hermes can also act as a client for viewing Relibase+ files. On Windows, your browser should be automatically configured by the CSD installer to open Relibase+ files. For Safari on Mac OS X there is no helper mechanism to automatically open downloaded files with Hermes. Instead you will need to download the file, then open it in Hermes manually. On Linux, on downloading a rlbcoor or reliview file from Relibase+ ensure that you choose the Open With option and choose `<INSTALLDIR>/GoldSuite_2017/bin/hermes`.

To start Hermes or GOLD, please refer to the instructions given in earlier in this section.

10.4.1 Testing your Installation

A number of tutorials are included with the GOLD Suite software. To test your installation and to learn something about the features of the software, it may be useful to try one or more of these tutorials which are located in the examples sub-directories of each GOLD Suite product.

Tutorial 1 involves PDB entry 1ACM. This is aspartate carbamoyl transferase complexed with a phosphonated, polar peptide ligand.

To use GOLD to dock the peptide ligand into aspartate carbamoyl transferase perform the steps outlined in the GOLD documentation for Tutorial 1.

The top level of the HTML version of the documentation can be found in the `docs` subdirectories of each GOLD Suite product.

10.5 Registration of CSD System Components

The CSD System Installer will offer you the opportunity to register the CSD System as part of the installation process, either by accessing our online registration servers, or by entering details of an existing and valid licence file. Registration online will require your Site Code and Confirmation Code.

If a valid licence is not present, then when using any component of the CSD System software (i.e. ConQuest, Mogul or IsoStar client) for the first time you will be prompted to register.

For more information about registration and licensing (see CSD System Software Licensing).

Mercury 3.9 and enCIFer 1.5.2 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 users.

10.6 Configuration of CSD System Components

10.6.1 ConQuest

Search Data Directory

Before using ConQuest 1.19 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 1.19 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 1.19 this file will be called `as538be.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 1.19 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 a PDF reader, such as Adobe Acrobat Reader. Adobe Acrobat Reader is available from the Adobe web-site: *http://www.adobe.com*. Other free PDF readers are available, see https://pdfreaders.org

10.6.2 Mogul

Database Location

Before using Mogul 1.7.2, 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 1.7.2 this file will be called `mogul538.path` and will be found in the data subdirectory in the location where you installed the database files.

10.6.3 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 Registering the Different Mercury Components).

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

Setting the `CSDHOME` environment variable on Linux and Mac OS X can aid in the location of the CSD software and data installation if you have a non-standard setup. Additionally, adding `<INSTALLDIR>/CSD_2017/bin and <INSTALLDIR>/GoldSuite_2017/bin`

to your `PATH` on linux can allow you to start the CSD software without use of the full path to its location.

For example:

1. To set CSDHOME for Bourne shell (sh) or Korn shell (ksh), type:
   ```
   CSDHOME=<INSTALLDIR>; export CSDHOME
   ```
   where `<INSTALLDIR>` is the top level CCDC directory of your CSD System installation.

   > For example:
   > ```
   > CSDHOME=/usr/local/CCDC/CSD_2017; export CSDHOME
   > ```
   > Or
   > ```
   > CSDHOME=/Applications/CCDC/CSD_2017
   > ```

2. Similarly, to set `CSDHOME` for C-shell (csh), type:
   ```
   setenv CSDHOME <INSTALLDIR>
   ```

   For example:
   ```
   setenv CSDHOME /usr/local/CCDC/CSD_2017
   ```

3. To add `<INSTALLDIR>/CSD_2017/bin` and `<INSTALLDIR>/GoldSuite_2017/bin` to your `PATH` for Bourne shell (sh) or Korn shell (ksh), type
   ```
   PATH=<INSTALLDIR>/CSD_2017/bin:<INSTALLDIR>/GoldSuite_2017/bin:
   $PATH; export PATH
   ```

4. Or for C-shell (csh) type:
   ```
   setenv PATH
   <INSTALLDIR>/CSD_2017/bin:<INSTALLDIR>/GoldSuite_2017/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`.

10.8   Unity desktop launchers for Ubuntu Linux

The CSD software now installs .desktop files suitable for use with the Unity desktop's launcher mechanism.

The files are installed into the CSD_2017/desktop and GoldSuite_2017/desktop directories of your linux installation for the respective programs that can be launched from the CSD software in those locations.

To associate a CCDC application with the Unity Launcher, use the command '`sudo desktop-file-install application.desktop`', which will require your account to be able to run commands as root via sudo. For example, to add IsoStar use:

```
sudo desktop-file-install isostar.desktop
```

Once done, you should find that application now appears as a searchable application to launch in the Unity interface.

In order to allow the 'Open With' dialog in browsers on Ubuntu 16 to offer IsoStar or Hermes as options when viewing IsoStar scatterplots or Relibase entries, this step will be required with the isostar.desktop and hermes.desktop files respectively.

See https://help.ubuntu.com/community/UnityLaunchersAndDesktopFiles for more details.

11 CSD Python API

The 2017 release of the CSD System software now includes a version of the CSD Python API and a distribution of miniconda Python in order to allow for easy use. This will be automatically installed together with the CSD software.

11.1 Use of the CSD Python API in Mercury

The CSD Python API menu in Mercury allows the running of python scripts in an interactive manner, typically acting on the currently viewed structure. This menu should default to using the included miniconda python installed in `the Python_API_2017` directory alongside the CSD software. The **Options…** menu may be used to specify a different python installation, or clicking the **Default** button will return to using the bundled version of the API.

For more details on the use of the API in Mercury, please refer to the Mercury User Guide.

11.2 Use of the CSD Python API via the command line

The CSD Python API can also be used via the command line. The CSD System installer will setup some convenient shortcuts and/or scripts to allow you to start the API with the correct environment already set. More details on using the Python API can be found in the CSD Python API documentation.

11.2.1 Using the CSD Python API on Windows

A Python command prompt may be started via the 'CSD Python API' shortcut that will have been created on your desktop, or in the Windows Start Menu.

To run in an existing command prompt window, navigate to the `Python_API_2017\miniconda` directory and type 'python'.

11.2.2 Using the CSD Python API on Linux

Start a terminal and navigate to the `Python_API_2017` directory. To get a python prompt where the API can be used, run the 'run_csd_python_api' script. A python terminal should start, reporting Python version 2.7.12.

To set up the environment correctly in the terminal without starting Python, navigate to the `miniconda/bin` directory and type:

```
source activate
```

A (root) prompt should appear at the start of the command line prompt, indicating that the correct environment should have been created. The miniconda python is now the default to be started by just typing 'python'.

To go back to a normal terminal, type the following in the `miniconda/bin` directory:

```
source deactivate
```

11.2.3   Using the CSD Python API on Mac OS X

Open Finder and navigate to the `Python_API_2017` folder. To get a python prompt where the API can be used, double-click on the '`run_csd_python_api`' script. A python terminal should start, reporting Python version 2.7.12.

The `run_csd_python_api` script can also be run from a terminal.

To set up the environment correctly in the terminal without starting Python, navigate to the `miniconda/bin` directory and type:

```
source activate
```

A (root) prompt should be created, and the correct environment for Mac will now be set to allow use of python scripts that utilise the API. To deactivate, type:

```
source deactivate
```

11.3   Use of the CSD Python API with your own Python installation

The CSD Python API may be installed into your own Python installation via use of pip or conda package managers. This method of use is recommended only for expert Python users who are experienced with installing Python packages.

Please refer to the CSD Python API forum at https://www.ccdc.cam.ac.uk/forum/csd_python_api/ for details on how to obtain and install these packages.

12   CSD System Software Licensing

12.1   Licensing Overview

As more than one program requires access to the licence information, the licence file is preferentially stored in a centralised location, 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* file is located in the home directory of the user (/home/user on Linux /documents and settings/user on Windows XP, /users/user on Windows Vista/7/8/10), 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 Registration Overview).

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 IP-Based Licensing).

12.2   Registration Overview

CSD System software is licensed 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 1.19, Mercury 3.9, Mogul 1.7.2) on a particular machine that has not been registered you will be prompted to register the installation using the process described below.

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

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 Specifying an Existing Licence File).

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) as well as a valid email address. These codes are supplied in a communication accompanying this release (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 dialogue box (see Online Registration). If you access the internet via a proxy server, you can enter its details first via the proxy button.

4. If your machine is not connected to the internet or if online registration fails, you must register offline (see Offline Registration).

## 12.3   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.

12.4   Online Registration

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

If online registration is successful you will see the following dialogue box:
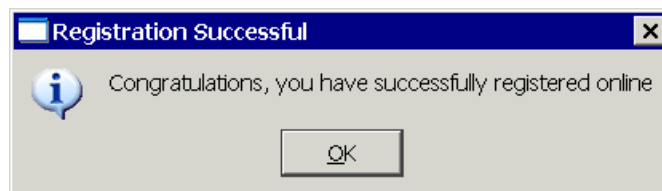
Note: When registering ConQuest, Mogul, or Mercury in this way it is possible to purchase additional licences online by clicking on the **Buy Additional Licences Online** button in the corresponding *Online Registration* window.

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.

- 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.

12.5   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:

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 336408

and a Validation Number will be issued to you.

12.6   Batch registration tool

The CSD Software installation now includes a batch registration tool that can be used to attempt on-line registration via the command line. This tool can assist in registration on servers where no display is present, or in automating the registration of installations across a site.

The batch registration tool will attempt to register the current machine online and append the resultant licence to csd_licence.dat in your current working directory. It is therefore advised to run the tool from the main CSD database directory, where it will be automatically picked up by all users. You will require write permission to the current working directory and csd_licence.dat file if one already exists.

The instructions below assume the database is installed in the default location – if located elsewhere then the command line instruction will require the correct path to the batch_register tool.

12.6.1   Windows

From `the CSD_2017\CSD V5.38` directory run:

```
..\Mercury\batch_register.exe -current_machine -site_id XXXX -
conf_code YYYYY -auto_accept_licence
```

12.6.2   Linux

From the `CSD_2017\csd` directory run:

```
../bin/batch_register  -current_machine -site_id XXXX -conf_code
YYYYY -auto_accept_licence
```

12.6.3   Mac OS X

From the `CSD_2017/DATA/CSD 538` directory run:

```
../../mercury.app/Contents/MacOS/batch_register -current_machine -
site_id XXXX -conf_code YYYYY -auto_accept_licence
```

12.6.4   Advanced Use of the batch registration tool

The batch registration tool may also be used in various other modes to facilitate registration on systems where online registration is not possible. For example, the tool can collect serial numbers of individual systems and store these in files in a single location. These files can then be used on a system that does have internet access to create a single licence file valid for all the systems where serial number data was collected.

To view the various options for the batch registration tool, run it with the `-help` argument. For help with batch registration please contact *support@ccdc.cam.ac.uk*.

12.7   Registering the Different Mercury Components

Accessing CSDS features:

- If Mercury 3.9 is started before the CSD software is 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 CSD-Materials and CSD-Discovery menus:

- Licensing of the CSD-Materials functionality of Mercury is handled through the existing CSD licensing system and the *csds_licence.dat* file. To register CSD-Materials in a copy of Mercury where it is currently not activated, select the **Register CSD-Materials...** option from the *Help* menu. Registration can be completed both online and offline as described above for the CSD System.

- Licensing of the CSD-Discovery accessible components of Mercury is handled in much the same manner. To register CSD-Discovery in a copy of Mercury where it is currently not activated, select the **Register CSD-Discovery...** option from the *Help* menu.

- A CSD-Enterprise licence will allow access to both CSD-Materials and CSD-Discovery components.

The **Help, About Mercury...** menu option will display details about your current licensing status, including CSD-Materials and CSD-Discovery.

12.8 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:

```
<INSTALLDIR>/CSD_2017/csd/csd_licence.dat
```

Mac OS X:

```
<INSTALLDIRDIR>\CSD_2017\DATA\CSD_538\csd_licence.dat
where <INSTALLDIR> is, e.g., \Applications\CCDC
```

Windows:

```
<INSTALLDIR>\CSD_2017\CSD V538\csd_licence.dat
where <INSTALLDIR> is, e.g., C:\Program Files (x86)\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.

12.9   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 licence file: (e.g. `<INSTALLDIR>/CSD_2017/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 Linux 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**.

12.10   Current Licence Information

It is possible to look at your current licence usage and allowances via the **Help, Current Licence Information** option in ConQuest.

The resultant page is divided into 2 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

13   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 2.2.4 client package.

14   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/data_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:
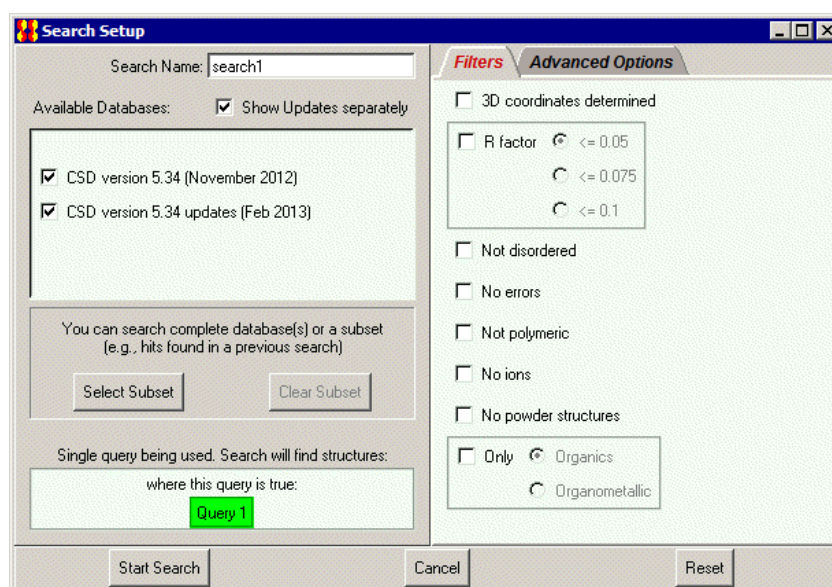
15 Activating In-House Databases

ConQuest 1.19 can search in-house databases in addition to the main CSD. These databases are created using the PreQuest program. If you have created an in-house 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 V5.38 database files. On Linux this is typically:

        <INSTALLDIR>/CSD_2017/csd

While on Windows, this is normally:

        C:\Program Files (x86)\CCDC\CSD_2017\CSD V538

And on Mac OS X:

        /Applications/CCDC/CSD_2017/DATA/CSD_538

You must then run the Activate program.

   1. For Linux, ensure that <INSTALLDIR>/CSD_2017/bin is in your PATH and type:

        activate

To run the *activate database* program on Windows select:

   Programs -> CCDC -> CSD System Software 2017-> Activate in-house database

from the Windows Start menu.

On Mac OS X, start a terminal window and run the command:

        /Applications/CCDC/CSD_2017/conquest.app/Contents/Resources/bin
        /activate

Note: Windows Vista/7/8 and 10 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 all cases a pop-up window like the one shown below will be displayed:
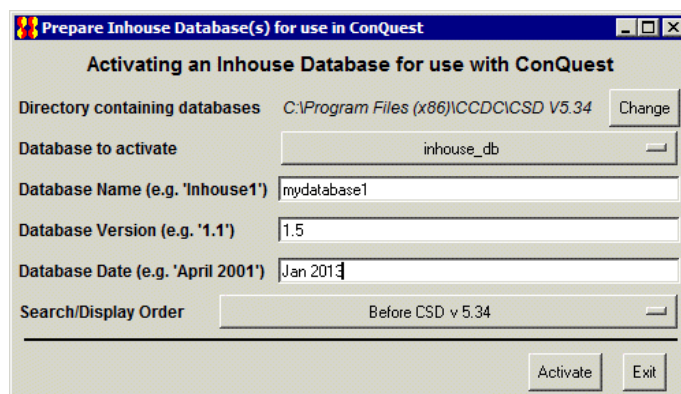
The activation program attempts to find the directory where the database is located by examining your ConQuest defaults file. However, if the correct directory cannot be found then use the **Change** button to locate the required directory.

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 v5.38,** 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.

16   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.

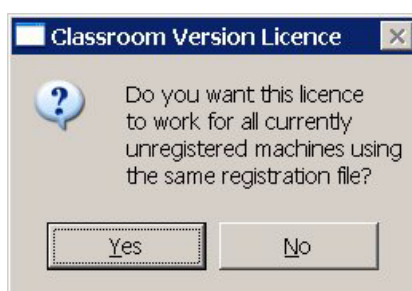## 16.1   Installing Classroom ConQuest

It is possible to register ConQuest 1.19 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*
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.

16.2   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:
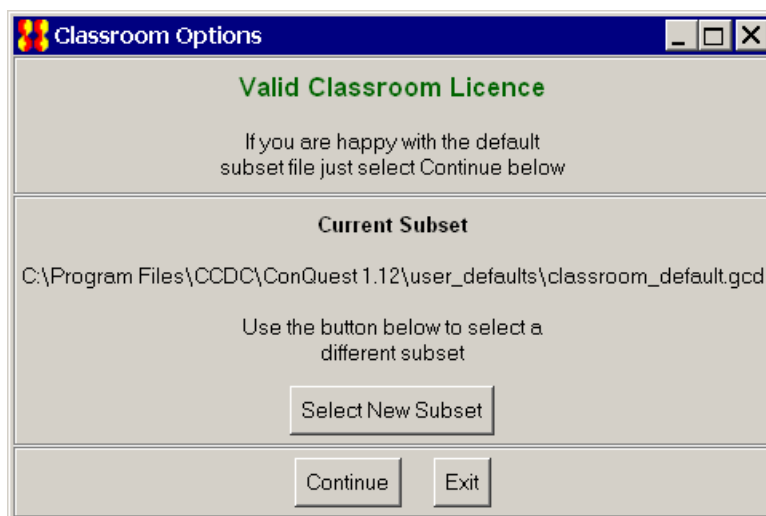

The aim of this dialogue box is to:

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

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.
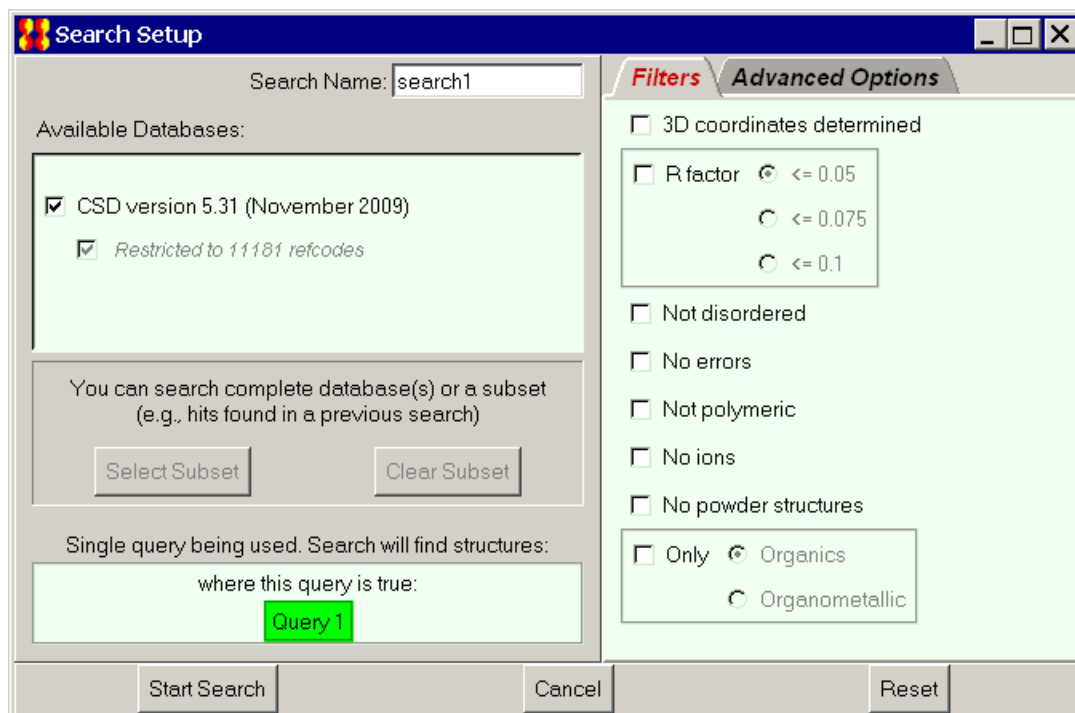
16.3   Choosing a Subset

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 Basics of Using Classroom ConQuest).

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.