Accessing information on Inorganic and Organic crystal structures using the Chemical ICSD and CSD database systems

Part 1:

Accessing crystallographic information on *Inorganic* Structures from any platform

If you need instant access to all parameters of most inorganic crystal structures please use:

1) Goto the following link: http://cds.dl.ac.uk/icsd/

2) Enter username / password (check note in the end)

3) Click on "access database".

4) Enter your required search terms e.g Zn Cl2 (spaces between elements)

5) Select one or more of the results

6) Click on "Structure" Structure to see the structure

7) Click on Detail to export crystallographic information in a e.g. CIF file to your computer

Part 2:

Accessing crystallographic information on *Organic* Structures using a **Windows** platform.

Step 1:
You first need to install Hummingbird Exceed (XServer) and then set up all parameters according to

http://cds.dl.ac.uk/cgi-bin/faq/display?42+1+4

Step 2:

Close Exceed & Restart Exceed (which starts the xserver in the background)
(Hummingbird Exceed is in your programs menu)

Step 3:
You now need to download an ssh client e.g. Putty
http://www.putty.nl/latest/x86/putty.exe

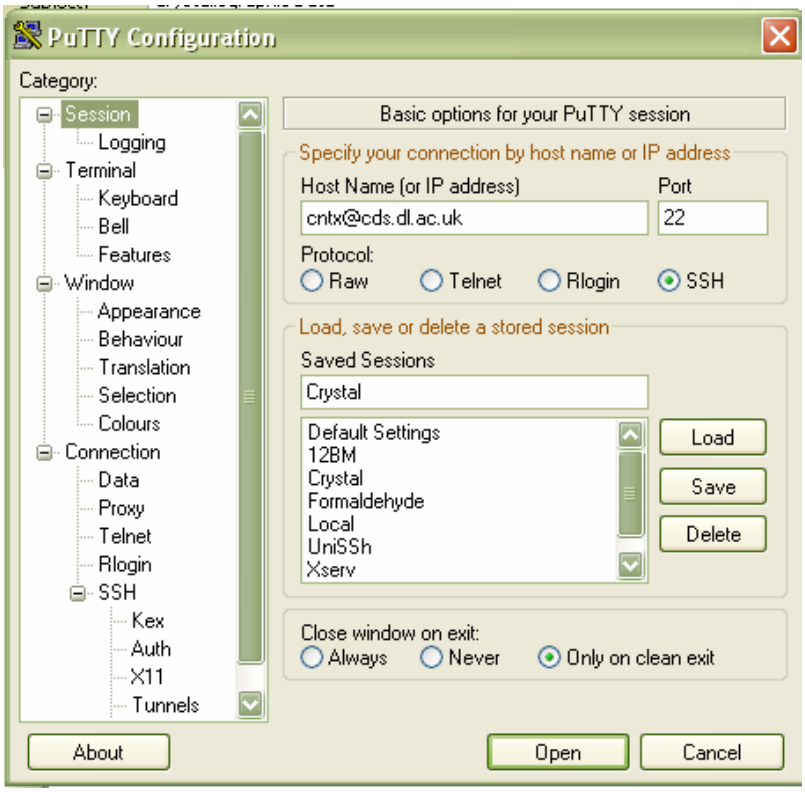
and also the file copy program e.g. PSCP
http://www.putty.nl/latest/x86/pscp.exe

download and save both files in C:\Putty\ and create a shortcut on your desktop

Step 4:

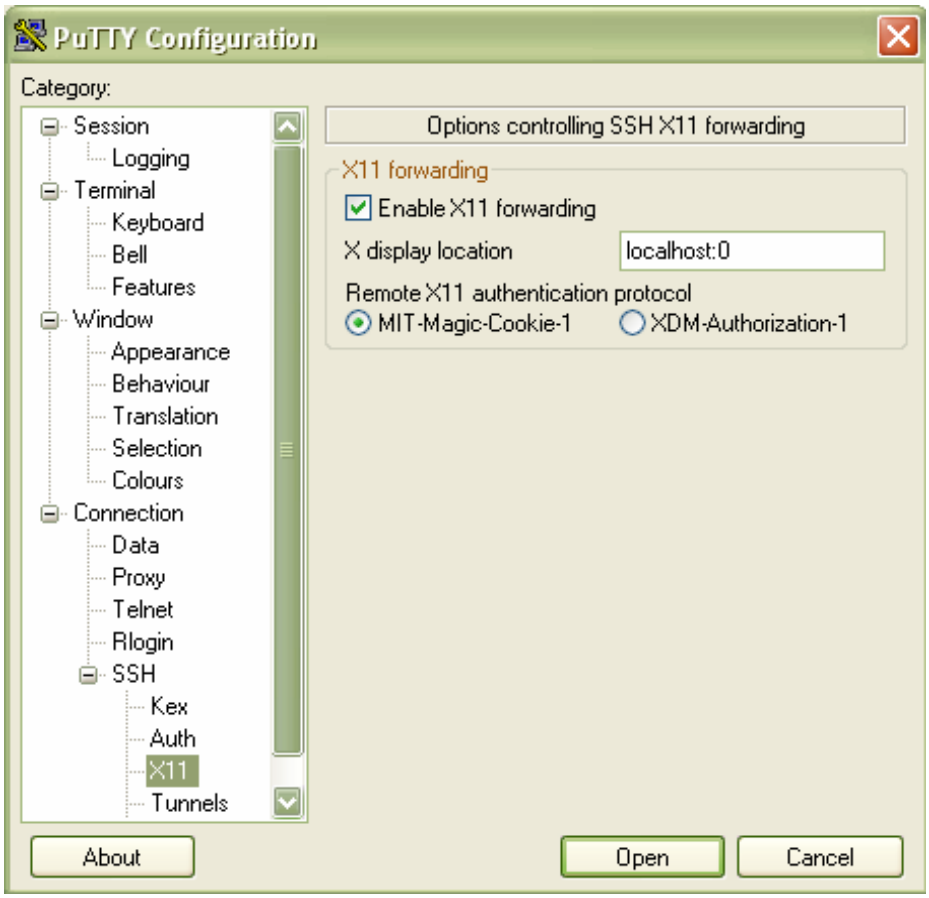
Start Putty.exe

Setup a ssh connection to cds.dl.ac.uk port 22.



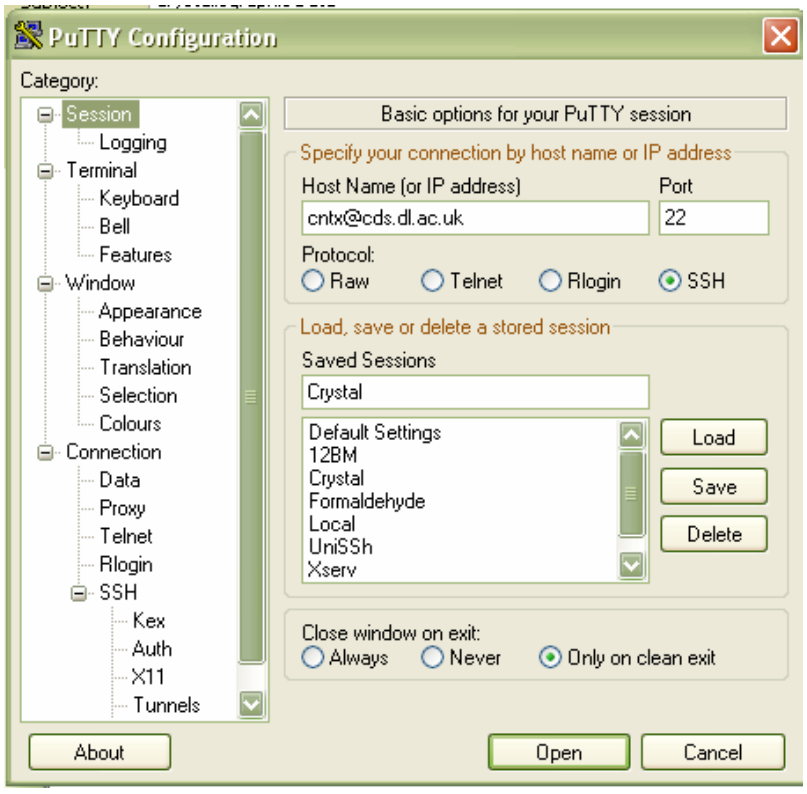
Step 4:

In Putty configuration goto the SSH : X11 selection and enter in the Xdisplay location “localhost:0”



Step 5:

Click on session and save the new connection as CrystalCSD or something.



Step 6:

Click on Open

and type your username and password (check note in the end)

Remember in Putty paste is right click

you should then come up with a similar screen as below.

Step 7:

type “xlogo“ and press enter

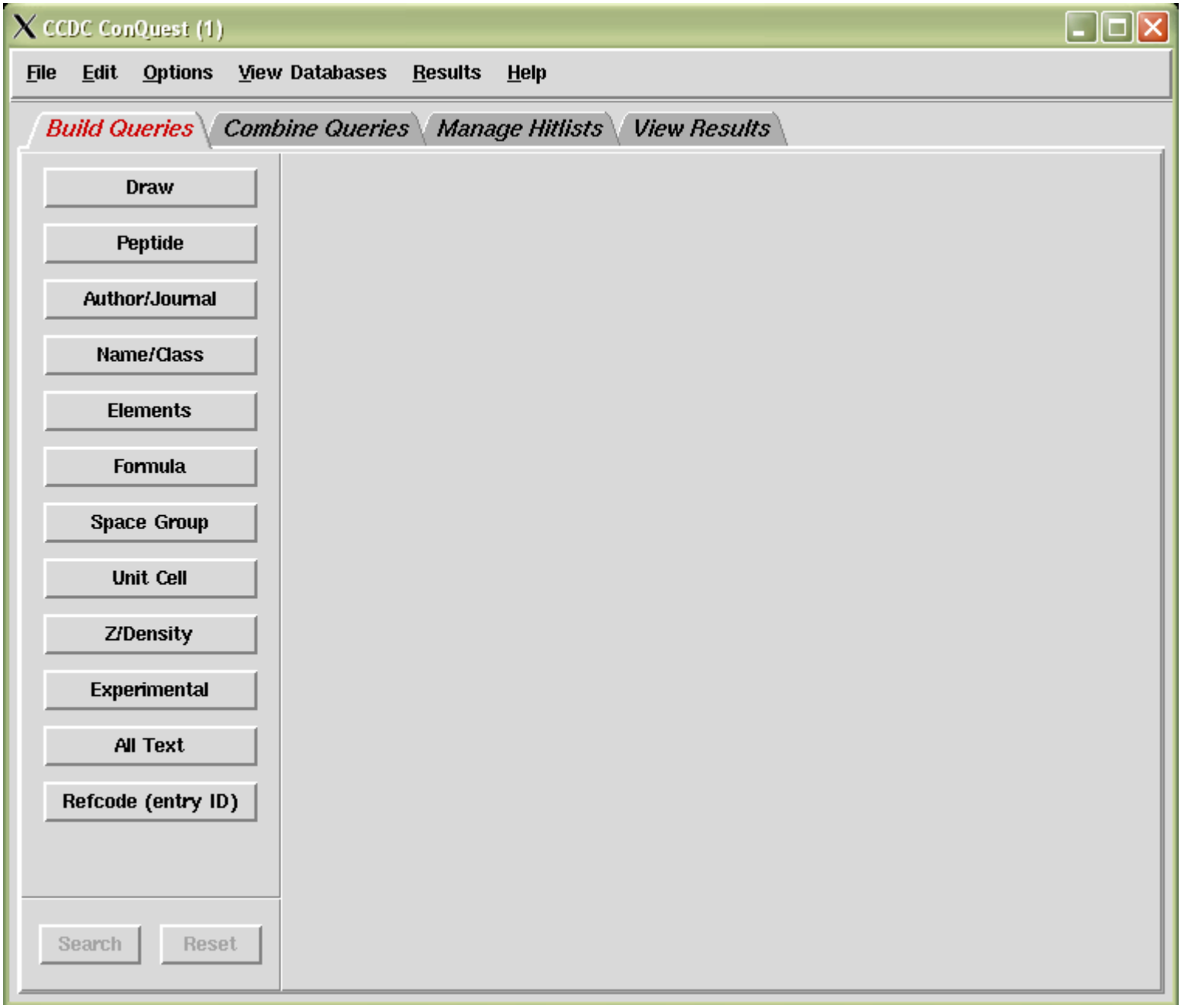
you should see the following snapshot

This basically verifies whether your xserver has started. If you don’t see this snapshot close putty and Hummingbird exceed and restart first exceed and then putty and then reconnect.

Step 8:

Now you are ready to start the Conquest engine just type conquest in the prompt.

Accept the User agreement and you should have the following screen available:



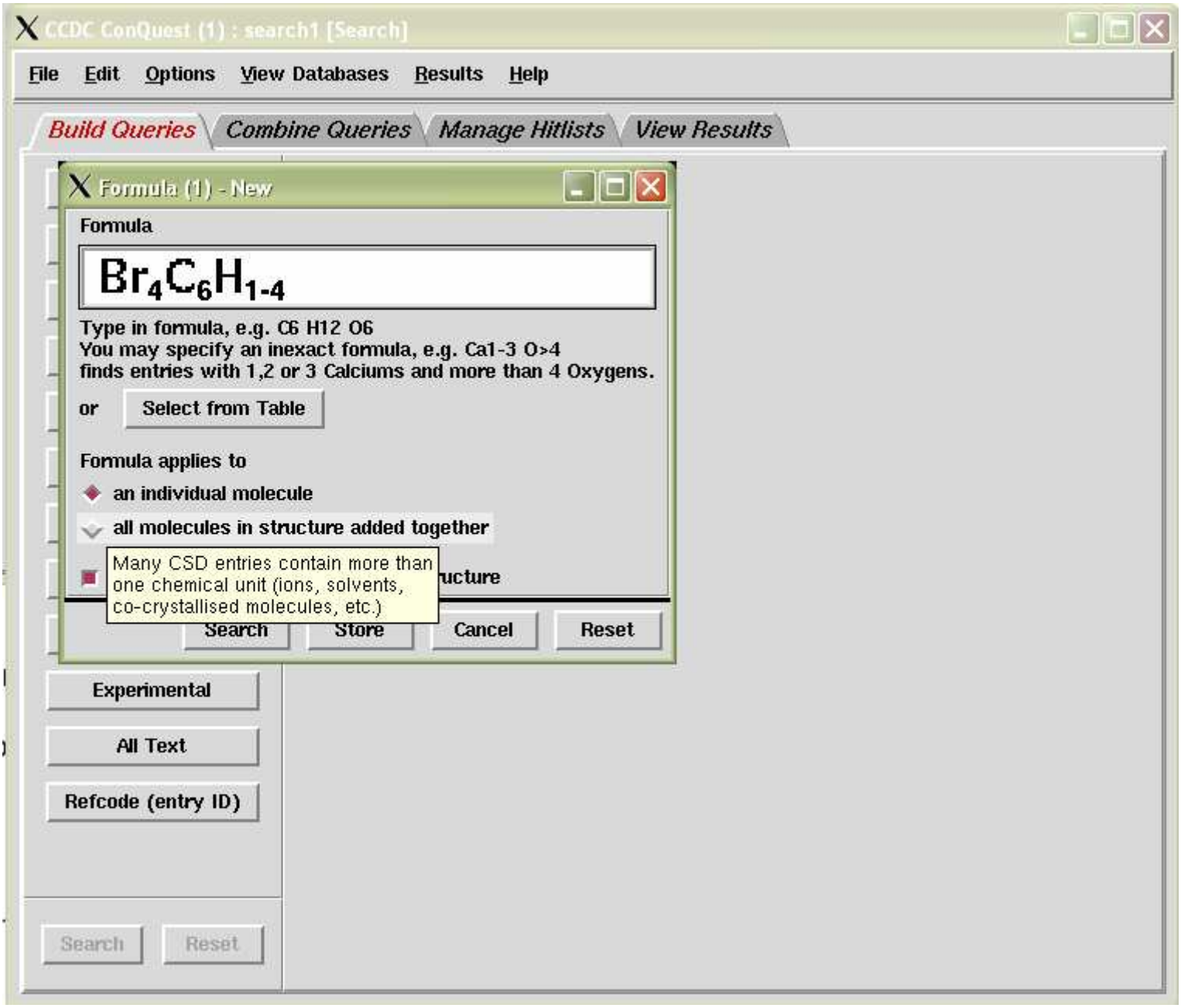
Info:
Conquest enables you to search the entire organic database with several different methods.
One of the most powerful facilities is the search by structure. This is where you can actually
draw a part of a structure and the super computer will find the best possible matches.

Step 9:
Quick Example, Search by formula:

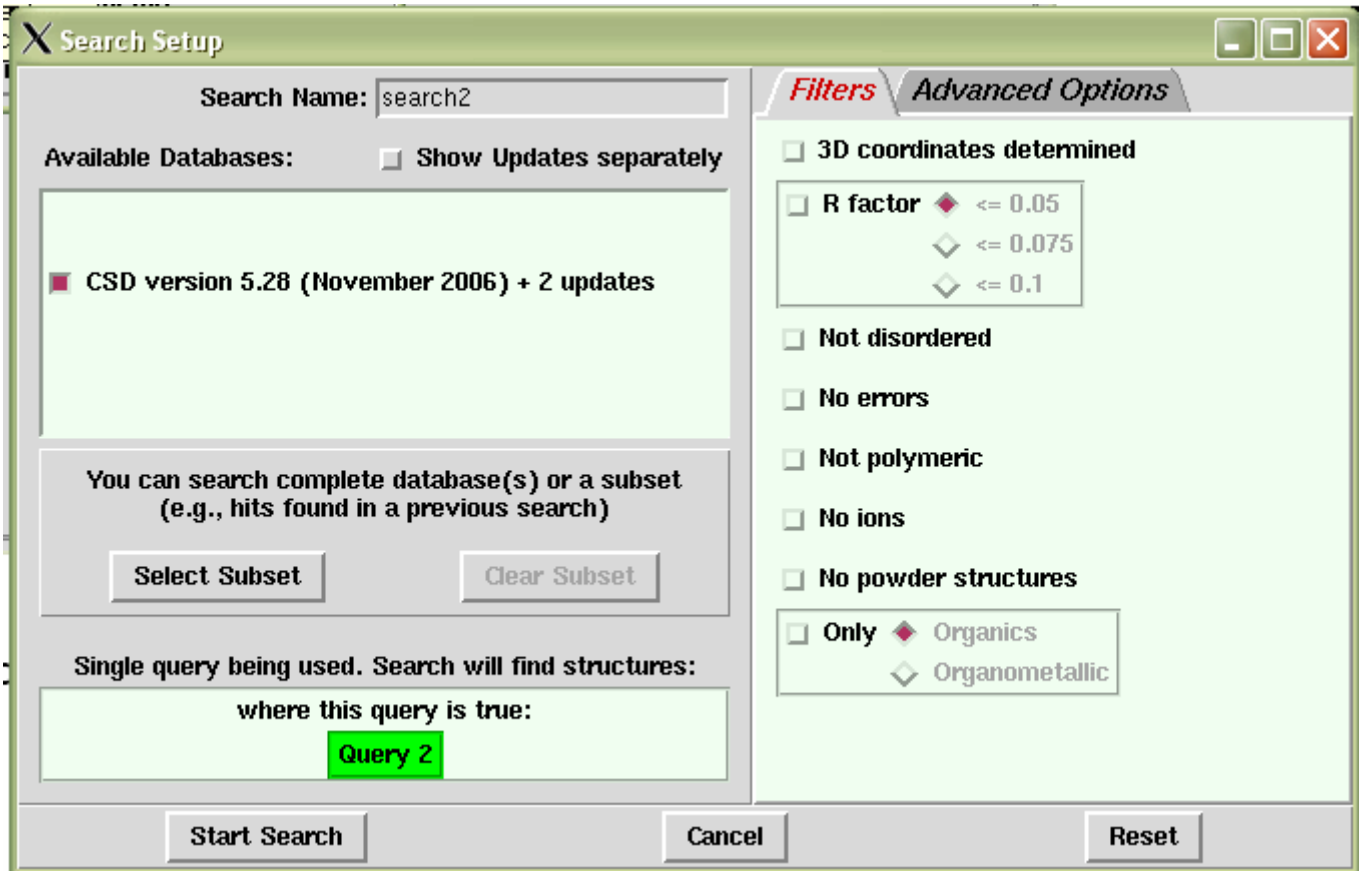
Click on the Formula button and enter

e.g: Br4C6H1-4

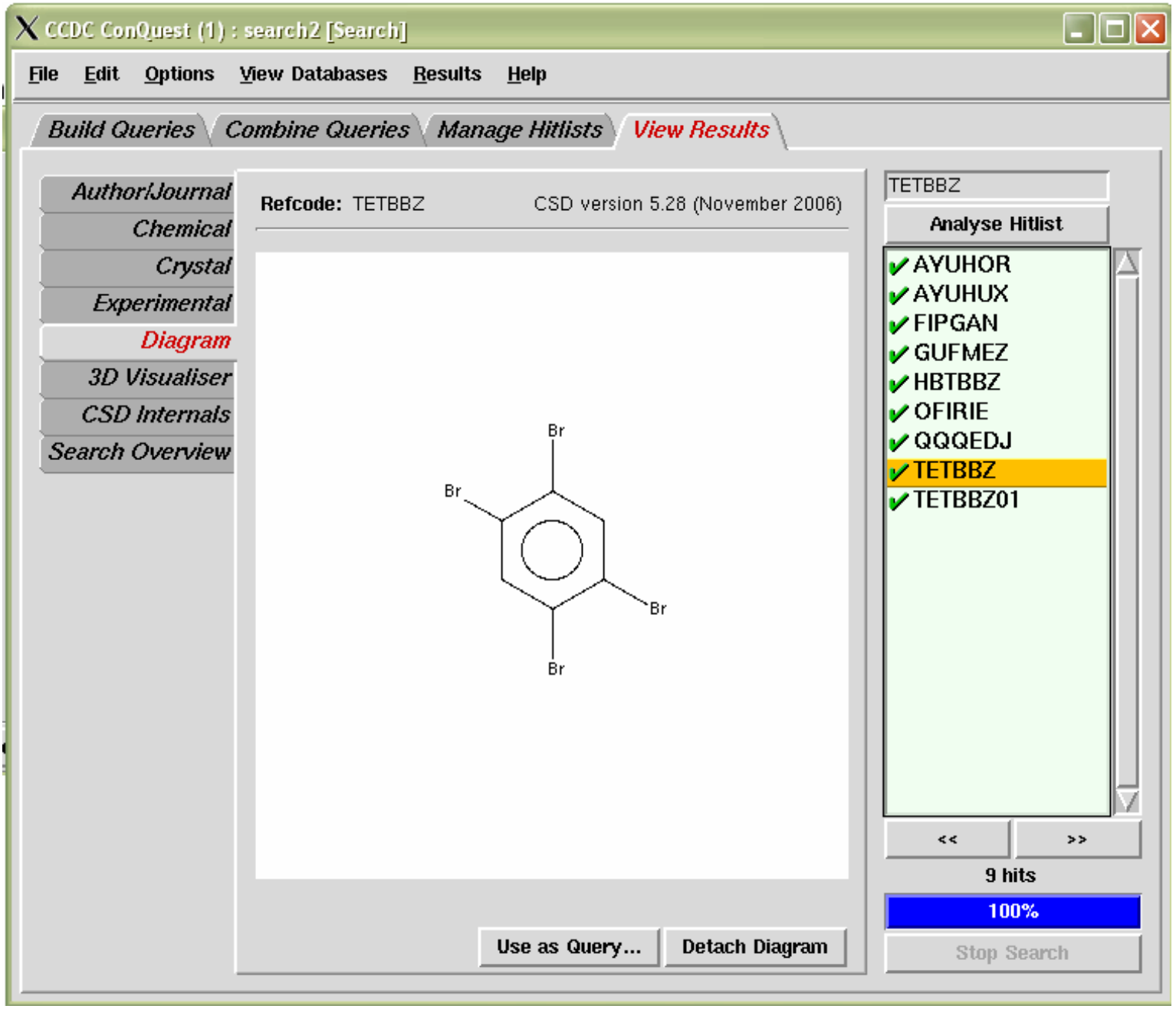
This will search for all possible structures with approximately 4 bromium, 6 carbon and 1,2,3 and 4 Hydrogen atoms



Click on the search button and you should see the following

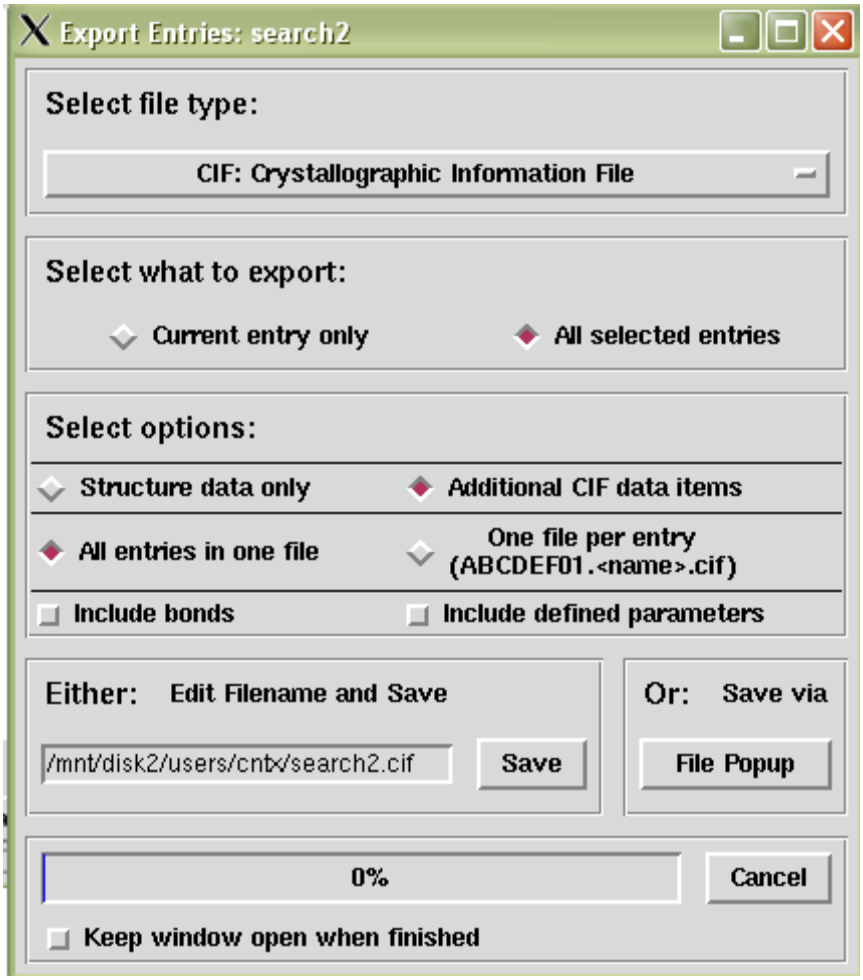


- Click start Search and after a few moments you should see all the possible structures.
- Scroll through to see the other available e.g hexabromobenzene etc
- And also in 3d by clicking on 3D visualiser (a bit slower though)
- Information on crystal structure is located under the Crystal button



Step 9:
Exporting the Structures

Click on File button and then the Export entries as button.
you should see the following screen.



- Select the file format. CIF is the standard format in crystallography and is accepted by most analysis packages.
  there are tens of other available formats

- Type the filename and location.(change only the name of the cif file e.g. search2.cif)

- Remember the location of the file is in a remote server so after you finish your search
  you have to download it in your computer.

- Click on the save button to save to the selected location

Step 10

Assuming you are finished with searching and saving the crystal structures

Downloading the remotely saved crystallographic data to your computer

1) Press the Windows and R button simultaneously.
2) Type in “cmd” and press enter.

You should now have the command prompt on the screen.

3) type cd c:\putty\ to go to the location of the pscp.exe and putty.exe programs

4) We will now download the remote file /mnt/disk2/users/cntx/search2.cif to your putty folder

type: pscp username@cds.dl.ac.uk:/mnt/disk2/users/username/search2.cif c:\putty\

or

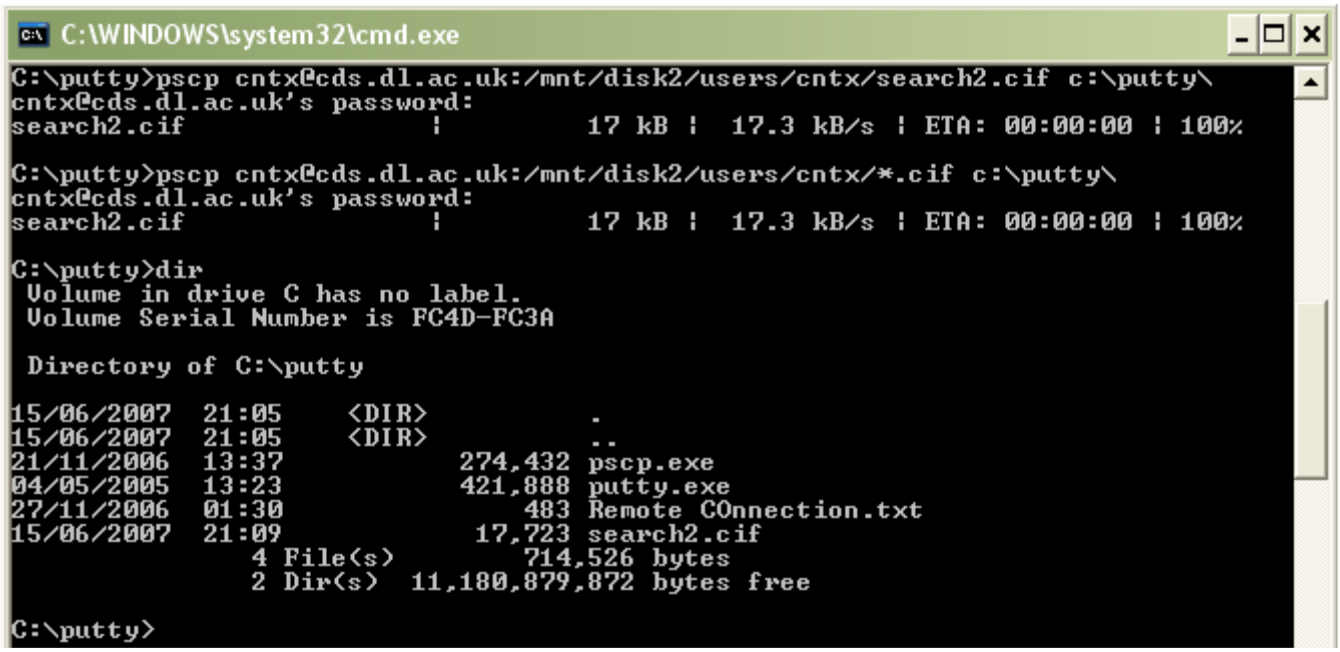
type: pscp username@cds.dl.ac.uk:/mnt/disk2/users/username/*.cif c:\putty\

…when you want to download all cif data files to your putty folder.

(where you see username you have to fill in your username.)

You will be asked for your password (then press enter).

You should see the following.



To verify type "dir" and then press enter to get a listing of the current directory.

Step 11:

From then onwards you can open the crystal .cif file with a myriad of programs.

Molpack, Mercury, iffefit, Artemis, Atoms, Gaussian, Feff82 …….

Notes:

1) You will need a single username and password to access both the ICDS, CDS databases.
It involves a registration process. Ask for details on the website and/or your supervisors.

2) For Linux users the process is largely simplified since the ssh client and xserver are already
integrated in the OS (follow from step 5 onwards). The remote file copy command is almost
identical just use scp instead of pscp

Links

http://cds.dl.ac.uk/cds/datasets/crys/csd/conquest/conquest.html

http://cds.dl.ac.uk/cds/interface_and_utilities/llinter.html

http://cds.dl.ac.uk/cds/interface_and_utilities/secureshell.html#putty

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