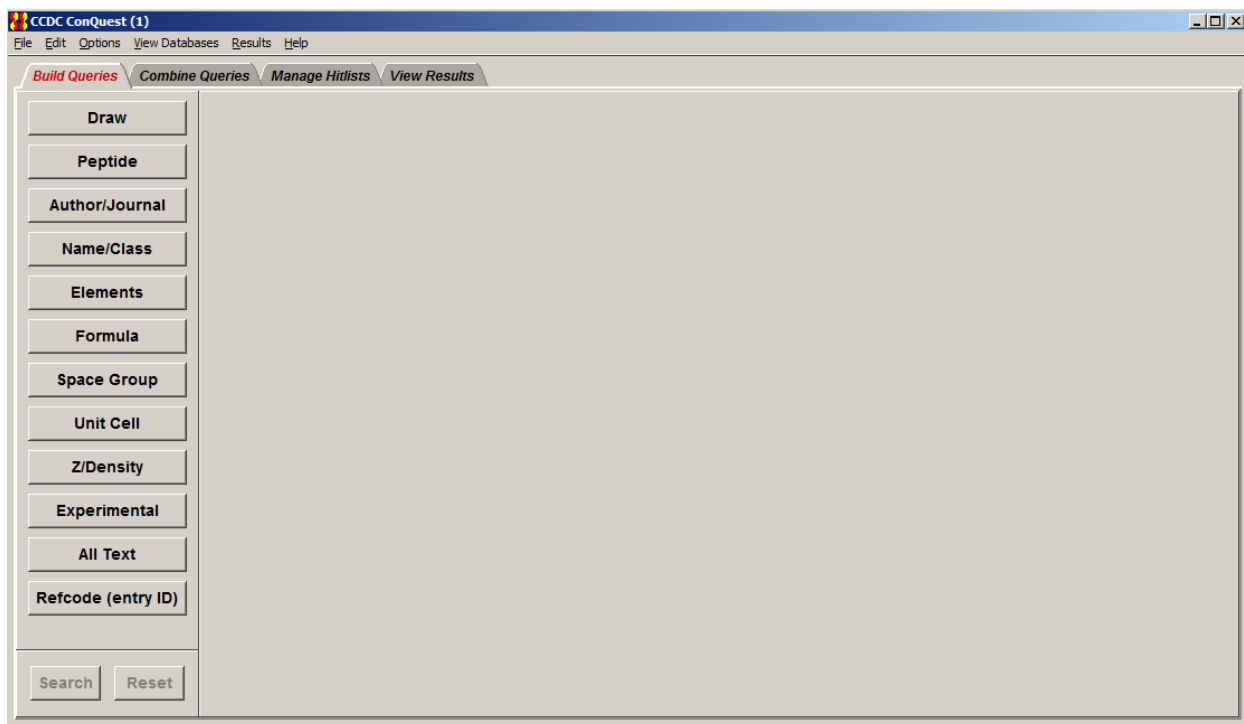


Databases

Databases

There are numerous databases that combine crystal structure information. Most of these databases are based on the type of molecule in the database and many contain overlaps. A highly useful database for the Department's Chemical Crystallography Laboratory is the Cambridge Structural Database, CSD, prepared by the Cambridge Centre for Crystallographic Data. This database contains all small-molecule organic and organometallic crystal structures ever published (except for the most recent ~ 6 months). Structures of polymeric compounds are usually limited to 10-12 residues. Currently there are over 900,00 structures listed in the database. <http://www.ccdc.cam.ac.uk/>

In our Laboratory, the CSD is only available on the computer XRAY5. The main program is opened with the "Conquest" icon on the desktop. The opening page appears below.

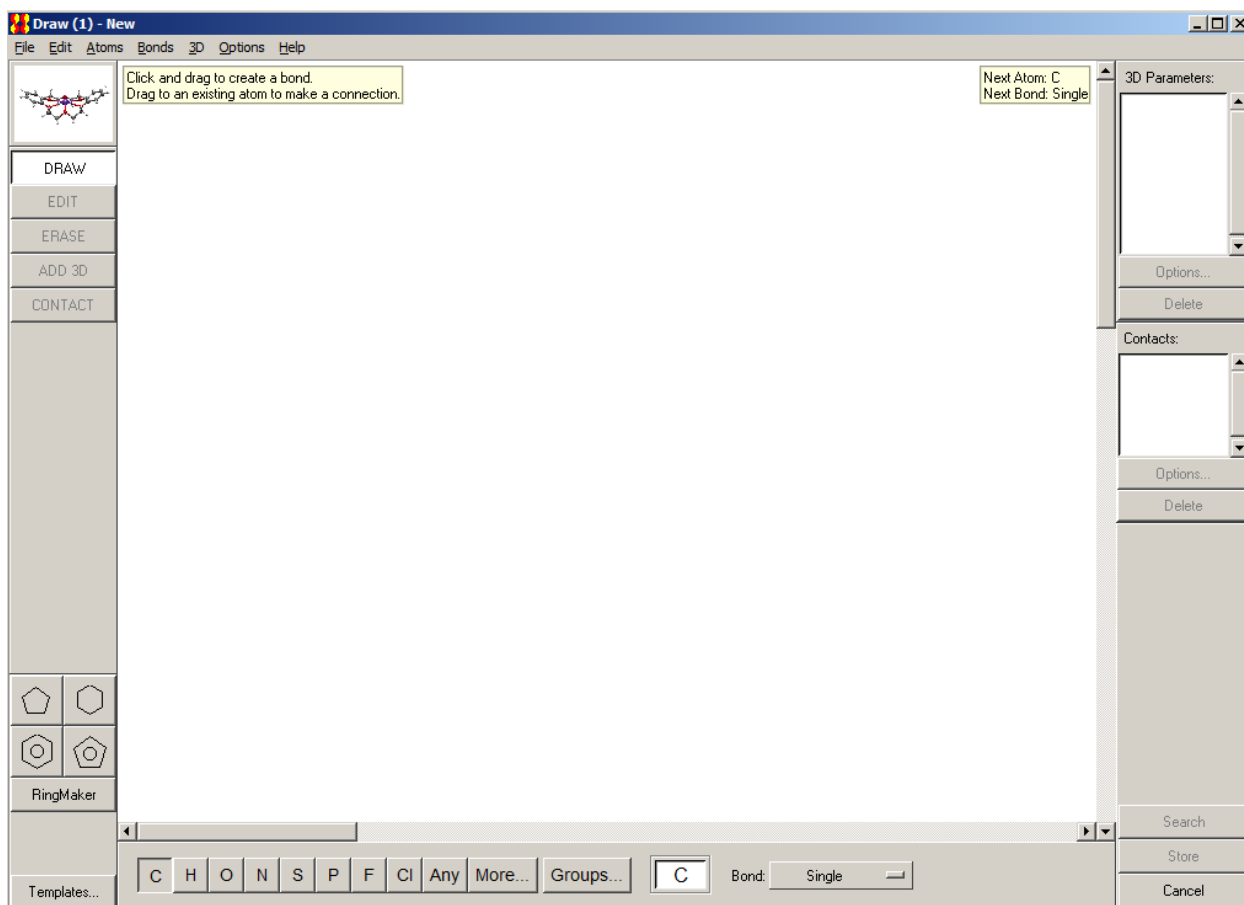


Search questions are called queries. This first page directs the user to the type of query they wish to construct. Users often want to search the database for some molecule or fragment of a molecule. Through the Author/Journal button, you can search for a specific article or related groups of articles. The Name/Class button does queries for these specific items but requires that the IUPAC name be known or that the class has been identified by either the original authors or the CSD. The Space Group button is good for statistics. The Unit Cell button often produces 40+ hits for nearly any cell. The Z/Density, Experimental, and All Text buttons are of limited use. Each entry is given a unique "Refcode". If the specific refcode is known, it can be located

with the Refcode button. Also note that multiple search questions can be saved and logically combined using “and”, “or”, or “not” type of logical operators in the Combine Queries menu.

The Draw menu contains a drawing screen with a list of common atom types on the bottom and all possible bonds. At the bottom left are menus to select rings and templates of common groups. Other atoms or groups of atoms can be selected from the “More” menu. When selecting the bond type, remember both a delocalized and an aromatic bond are of order 1.5. Delocalized bonds are not in a ring; aromatic bonds are in a ring.

There are two caveats about using this program. When your search yields no hits and the molecule can be in another conformation, e.g., as keto, enol conformers, then try searching for the other conformation. Second, when a metal is bonded to the pi system of an aromatic ring, draw only one bond between the metal and the ring.



When searching for an author’s name, the search should only contain the initials of the first and middle names and the last name, no capitals, and no spaces. When I search for my name I need to set up two queries, one for “d.powell” and another for “d.r.powell”.

In addition to the CSD database, the *free* Crystallography Open Database is available at <http://www.crystallography.net/cod/>

The structures of proteins are listed in the free Protein Data Bank, <http://www.rcsb.org/pdb/home/home.do> and the free Nucleic Acid Database, <http://ndbserver.rutgers.edu/>.

Inorganic Crystal Structures are given in the <http://icsd.ill.fr/icsd/>, the Pearson Database, <http://crystalimpact.com/pcd/Default.htm>, the free Mineralogy Database, <http://www.webmineral.com/>, and the free American Mineralogist Database: <http://rruff.geo.arizona.edu/AMS/amcsd.php>.

Powder diffraction data are available from the ICDD at <http://www.icdd.com/>.

Databases marked as free are available over the internet at the addresses shown. The department has access to the Cambridge Structural Database (courtesy of the CCL) and the Pearson Database (courtesy of the OU Library and Prof. Saparov).