i) The CrystalWeb database interface – Bob McMeeking & Dave Fletcher (r.f.mcmeeking@dl.ac.uk & d.a.fletcher@dl.ac.uk)

Ready access to the major crystallographic data collections has always been a key feature of the Chemical Database Service[1]. Locally written retrieval codes have been developed over the years to access the Cambridge Structural Database of organics and organometallics (CSD), the Inorganic Crystal Structure Database (ICSD), the Metals Data File (CRYSTMET) and the NIST Crystal Data Identification File (CDIF). At the same time the various data providers have been busy developing their own specifically tailored retrieval and analysis software packages[2], many of which are also available to users via CDS[3].

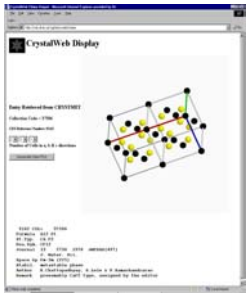
In all cases different, separate searches have to be performed on the various datasets. The "classic" CDS developed interfaces to CSD, ICSD, and CRYSTMET have core features in common, but are command-line driven, with limited graphics facilities and without the intuitive look and feel required of modern interfaces. The CDS interface to CDIF provides special facilties to perform unit cell searching which is not dependent on the choice of crystallographic setting selected. It is completely different from the other interfaces but is also command-line driven.

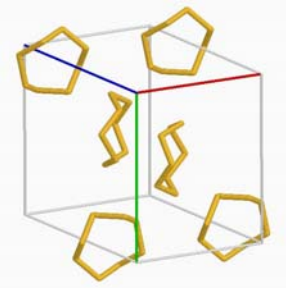
The CrystalWeb system has been developed to address these deficiencies. It uses Web Browser technology, performs searches over all datasets simultaneously, and has a common graphics display option giving good quality display facilities for all structure types. In addition there is direct "single click" access, using the LitLink system[4], to sources of the primary electronic literature where these are available.

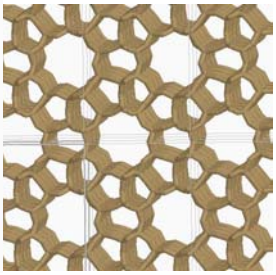
For CrystalWeb we extract the items from the disparate datasets and put them into a relational database management system. We use the well established Chime plugin (from MDL, based on RasMol)[5] to provide its molecular graphics capabilities. There is however no intention to try to emulate many features of existing excellent systems such as the CSD ConQuest & VISTA packages.

CrystalWeb already provides a range of search forms. Search items include bibliographic features such as authors and journals, chemical composition, and compound name. A CDIF-type search should be a prerequisite before embarking on most crystallographic refinement studies and the option within CrystalWeb to include all datasets is of particular value.

Data literature can be exported in a wide range of file formats. These include the classic .XR format familiar to established CDS users, SHELX, CIF, and a range of molecular modelling formats. The aim is also to support XML/CML formats in line with developments and emerging standards for the Semantic Web or GRID[6].







a) *TheCrystalWeb display window; details for SiO_2, Zeolite ZSM-11 from ICSD – there are links to LitLink, Chime display and the various file format Export options* ***b)*** *Chime display for $PtAl_2$ from CRYSTMET – there are facilities to specifiy multiply cells* ***c)*** *S_8 from ICSD – CrystalWeb generates unique molecules correctly in such systems* ***d)*** *The extended network structure for Zeolite ZSM-11.*

[1] "The United Kingdom Chemical Database Service", Fletcher, D.A., McMeeking, R.F., Parkin, D., *J. Chem. Inf. Comput. Sci.* (1996), **36**, 746-749.

[2] "Crystallographic databases – various articles", Edited Allen, F.H., Glusker,J.P.,*Acta Cryst*. (2002), **B58**, 317-920.

[3] Up-to-date information is available on the CDS Website; http://cds.dl.ac.uk

[4] LitLink is a software package produced by MDL Information Systems Inc. For further information visit http://www.litlink.com
[5] Chime is produced by MDL Information Systems Inc. For further information visit http://mdlchime.com

[6] For further details visit the the World Wide Molecular Matrix website; http://wwwmm.ch.cam.ac.uk