Prequest gives a friendly interface with which to check out the content of a CIF file, giving interactive graphic display of the 3D molecular structure. Messages are given if items normally expected in CSD entries are missing from the CIF.

Prequest also accepts other common formats such as SHELX. Cartesian coordinates from modeling or theoretical calculations may be input in MOL2 format. Fragments of proteins may be inserted from PDB format with automatic generation of connections and bond types. Generation of 2D chemical diagrams with bond-type from the 3D coordinates is provided, either automatically or by direct 2D drawing. Checks are made for matching of 2D/3D connectivity before storage.

For further details see http://www.ccdc.cam.ac.uk

**PS22.04.04 MULTIPLE ACCESSIBILITY TO THE THIRD DIMENSION IN CRYSTALLOGRAPHY**

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High-resolution crystallographic structures of metalloproteins often require the study of large molecular systems. Within the crystal, multiple molecules may be present, and the problem of establishing the relative orientation and conformation of these molecules can be very difficult.

The Inorganic Crystal Structure Database (ICSD) contains examples of simple and complex systems, and this paper describes recent additions of new structures to the database. In particular, the crystallography of bowl-shaped metalloproteins containing a large number of solvent molecules is illustrated.

**Databases II-Inorganic Materials, Powder Diffraction and Polymers**

**MS22.02.01 COMPUTATIONAL MATERIALS DESIGN: SYNERGY OF FIRST-PRINCIPLES CALCULATIONS AND EXPERIMENTAL DATABASES.**

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Progress in computational methods combined with the development of novel experimental techniques have created exciting opportunities for materials design. Both computations and experiments are generating data at an increasing rate. Thus, it is of utmost importance to define and implement comprehensive data models to accommodate these results and to create software systems which can operate on this wealth of information.

The first part of this contribution provides an overview of current theoretical and computational methods for the prediction of materials properties. A particular emphasis is on first-principles density functional methods, which have become truly remarkable tools for structural predictions for a wide variety of systems including organic molecules, organometallic compounds, semiconductors, metals, and ionic compounds.

In addition to giving structural information with an accuracy of a few hundredths of one Ångström, quantum mechanical methods generate detailed information on the electronic structure and related properties, which is usually complementary to the results of experimental methods such as x-ray diffraction methods, x-ray photoemission spectroscopy, scanning tunneling microscopy, and vibrational spectroscopies. This complementarity can be exploited for analytical purposes, for example in solving crystal structures. In the second part, the capability of present computational methods are illustrated in the context of semiconductors, inorganic pigments, and materials for energy storage. The third part provides an outline of a data model to capture both experimental and computational information. A perspective on emerging computational methods, computer technologies, and communications will conclude this contribution.