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## REMOTE ACCESS AND LABORATORY INFORMATION MANAGEMENT SYSTEMS (LIMS) FOR SINGLE CRYSTAL DIFFRACTION EXPERIMENTS

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The introduction of modern CCD X-ray detectors for single crystal diffraction has caused a tremendous change in everyday laboratory life. Data collection can now be accomplished within minutes to a few hours using sensitive CCD detectors. Single Crystal facility managers are faced with large amounts of data being collected and analyzed. Management of these data has become a major task besides the crystallographic work which has to be accomplished. Interfacing of the data acquisition and data processing programs to a LIMS in combination with remote access to the experiment can dramatically improve productivity. For a home lab remote access it offers convenience: control from the office, while the instrument is located two floors beneath. Within a university members of a remote institute can run their experiments themselves and do not depend on valuable local operator resources. Bruker Nonius has expanded this strategy of remote control even between different universities. Small departments benefit from the possibility of sharing an instrument between several groups. In some cases, such collaboration was essential to get funding. A LIMS will help to organize data and parameter storage, secure remote access to information as well as allow the use of electronic signatures required by CFR 21 part 11. A network connection is used to establish the remote access to the instrument from a control computer. This computer is used for data collection, data integration and structure solution. The concept of remote access and interfacing of data acquisition and processing software to a LIMS will be presented.

**Keywords: REMOTE ACCESS LABORATORY INFORMATION MANAGEMENT LIMS**

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## ARCHIVING ACTIVITIES OF THE PROTEIN DATA BANK AT OSAKA UNIVERSITY

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The Protein Data Bank (PDB) is the sole international repository for three-dimensional data of biological macromolecules and is managed by the Research Collaboratory for Structural Bioinformatics (RCSB), USA. The RCSB is a consortium composed of Rutgers University, the National Institute of Standards and Technology, and the San Diego Supercomputer Center. PDB entries are deposited via Web-based tools over the Internet at three sites, Rutgers University, European Bioinformatics Institute and Osaka University, in the world. The deposited PDB entries are annotated and processed at each site and then are combined at Rutgers University.
The Institute for Protein Research, Osaka University, Japan started to serve as the deposition and processing center of PDB entries on July 1, 2000 for crystallographers and NMR spectroscopists in Asian and Oceanic regions. Since then, we have collected and processed a total of 533 PDB entries as of February 26, 2002. We operate ADIT (**http://pdbdep.protein.osaka-u.ac.jp/**), a Web-based PDB input tool and the same one used by the RCSB. We have now four PDB annotators.
The PDB activities at Osaka is now operated by the PDBj (The protein Data Bank of Japan, **http://pdbj.protein.osaka-u.ac.jp/**) and have been supported by grants ACT-JST and BIRD-JST from Japan Science and Technology Corporation.

**Keywords: PROTEIN, DATABASE, CRYSTAL**

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## SOFTNESS SENSITIVE BOND VALENCE MODELS FOR STRUCTURE - CONDUCTIVITY CORRELATIONS IN SOLID ELECTROLYTES

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Established bond valence (BV) parameters rely on the assumption that the BV sum of a central ion is fully determined by interactions to counterions in its first coordination shell. The resulting small range of bond lengths led to the unphysical postulation of a universally fixed value of the BV parameter b that characterizes the shape of the BV pseudo-potential for the atom pair. However, recent applications of the bond valence concept, e.g., to model ion transport pathways in solid electrolytes, demand sensible estimates of the bond valence sums for mobile ions at interstitial sites and bottle-necks of transport pathways. BV calculations for these non-equilibrium sites require the knowledge of the actual shape of the BV pseudopotential. A systematic route to the determination of bond softness sensitive BV parameters for main group halides and chalcogenides from reference structures in the ICSD database is developed using an empirical correlation between b and the absolute softnesses of the interacting particles (cf. **http://kristall.uni-mki.gwdg.de/softbv/index.html**). With the help of softness sensitive BV parameters the crystal chemical information in the structure database has been effectively utilized to improve the quality of local structure models from reverse Monte Carlo (RMC) fits to diffraction data and to analyze ion transport pathways in glasses. From the volume fraction of regions with a sufficiently low valence mismatch for the respective mobile ion both absolute value and activation energy of the ionic conductivity can be predicted for a wide range of ion conducting glasses with various mobile ions (including mixed alkali systems).

**Keywords: BOND VALENCE IONIC CONDUCTORS REVERSE MONTE CARLO**

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## THE USAGE OF DATABASE TECHNIQUES TO EVALUATE THE STRUCTURAL GENOMICS TARGETS

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The ultimate goal of the Protein Structure Initiative (PSI) is to cover the entire protein structure space. The Structural Genomics Centers exploit the available genome sequence information to select targets for structure determination. Selection of targets for structural genomics studies is very important as determination of each new 3D structure may offer not only insight into its function, but also into the function of all sequence homologs. Moreover, many related structures can be determined using homology modeling methods. The information about structural genomics targets is dynamical and any analysis has to be provided on-line with the use of database techniques. Current analysis of all target lists from Structural Genomics Centers shows that there are 14571 targets, among which 12884 are non-redundant. Since 10761 targets have sequence identity lower than 30% to structures already deposited in the PDB, comparative model building based upon structures of these targets may provide additional space coverage for proteins with sequence identity >30% to them. An analysis of the quality of structures obtained initially from PSI will be presented and compared against structures available in the PDB.

**Keywords: MACROMOLECULAR CRYSTALLOGRAPHY BIOINFORMATICS DATABASE**