STAR ONTOLOGIES: KNOWLEDGE RETENTION THROUGH FUNCTIONAL RELATIONSHIPS

S.R. Hall[1] D. du Boulay[1] I.R. Castleden[2] N. Spadaccini[2]
[1]University of Western Australia Biomedical & Chemical Sciences Stirling Hwy NEDLANDS WA 6009 AUSTRALIA [2]School of Computer Science & Software Engineering, University of Western Australia, Nedlands 6009, Australia

A key objective for databases is to delineate and capture computer-interpretable "knowledge" (i.e. meta-data) from non-derivative information (e.g. postulates and measurements) so that data can be modelled as part of a database validation and mining process. Current data handling approaches based on customized software are inflexible because they cannot respond quickly to changing methodologies. They are also difficult to extend so as to prevent the seamless addition of new data types and structures. Anther fundamental weakness is that software-encoded knowledge, which is usually encrypted in an imperative language, is neither easily human-accessible nor re-useable – and this inhibits knowledge retention, knowledge evolution and direct pedagogical applications.
This talk will describe a generic approach to coalescing meta-data into domain-specific ontologies in which methods expressions, written in a symbolic text language dREL, describe complex relationships between defined data items [1]. A parser-compiler converts ontologies into a series of Java objects, forming an executable knowledge kernel for data manipulation, validation and interpretation tools. A prototype crystallographic ontology, based on the Core CIF dictionary, will be used to demonstrate the evaluation of derivative data and the redefinition of enumeration states.
References
[1] Spadaccini, N., Hall, S.R., and Castleden, I.R. "Relational Expressions in STAR File Dictionaries" 2000 J Chemical Information and Computer Science 40, 1289-1301.

Keywords: DATABASE KNOWLEDGE ONTOLOGY DEFINITION DATA VALIDATION

CRYSTAL STRUCTURE PREDICTION BY DATA MINING

D.W.M. Hofmann[1] T. Lengauer[2] J. Apostolakis[3]
Fhg-Scai. Alg Schloss Birlinghoven ST. AUGUSTIN D-53754 GERMANY [1]University Bonn, Department of Informatics [2]Max-Plank-Institut Fur Informatik, Saarbrucken [3]Fraunhofer-Institute for Algorithms and Scientific Computing, Sankt Augustin

The ever increasing number of experimentally determined crystal structures allows for the use of data mining methods, to address crystallographic questions. Here we study the application of data mining for predicting the arrangement of molecules in unit cells of unknown dimensions (crystal structure prediction).
In this work, data mining is used to derive an atom-pair potential, which is then compared to known force fields. It is shown that the potential is physically reasonable when the data are sufficient in quality and quantity. For validation the energy function is applied to the problems of crystal structure prediction and fractional coordinate prediction. In both cases a large number of structures was generated and the structures were ranked according to their energies. Structure prediction was considered successful if a structure similar to the experimentally observed one was ranked highest.
For crystal structure prediction the energy function is tested on an independent set of crystal structures taken from the *P*1 and *P*-1 space groups. We show that approximately 76% of the 218 molecules tested in space group *P*1 are predicted correctly. for the more complex space group *P*-1 the success rate is 24%.

Keywords: DATA MINING, TRAINED POTENTIALS, CRYSTAL STRUCTURE PREDICTION

STRUCTURE AND PROPERTIES OF LEAD CARBOXIPHOSPHONATES HYBRID MATERIALS

A. Cabeza[1] M.M.G. Alcantara[1] M.A.G. Aranda[1] J.G. Mao[2] A. Clearfield[2] A. Guagliardi[3]
[1]Universidad De Malaga Quimica Inorganica C/ Teatinos S/N MALAGA 29071 SPAIN [2]Texas A & M University, College Station, Texas, USA [3]C.N.R. - Irmec, Bari, Italy

Metal phosphonates are organo-inorganic hybrids which have received considerable interest in the last decades. They show a wide variety of potential applications as well as diverse structural types: one-dimensional chains, layered and three dimensional microporous frameworks. The use of diphosphonic acids [$(HO)_2OP$-R-$PO(OH)_2$] and carboxialkylphosphonic acids [$(HO)_2OP$-R-COOH] have shown a great interest because the careful selection of the R groups will be able to control some important characteristics of these materials such as interlamellar distance, pore size, and even its potentially shape selective properties within a controllable structure. In this work, we present the crystal structure of two new lead carboxiethylphosphonates hybrid materials:
$Pb_3(O_3PCH_2CH_2COO)_2$ and $Pb_5(O_3PCH_2CH_2COO)_2(O_3PCH_2CH_2COOH)_2$. Both compounds were prepared under hydrothermal conditions using different Pb/Phosphonic acid molar ratios. Firstly, $Pb_3(O_3PCH_2CH_2COO)_2$ crystallizes in a monoclinic cell with parameters a = 10.72 Å, b = 14.55 Å, c = 9.05 Å and β = 111.18º, V = 1317 Å^3. Its structure was solved by *ab initio* powder diffraction method and refined with GSAS using the Rietveld method, RWP = 0.086 and RF = 0.041. The framework is layered where both carboxylic and phosphonate groups are bonded to the leads. There are three different lead atoms showing distorted oxygen environments due to the lone pair. Secondly, $Pb_5(O_3PCH_2CH_2COO)_2(O_3PCH_2CH_2COOH)_2$, is also monoclinic with a = 11.88 Å, b = 12.75 Å, c = 9.83 Å and β = 114.08º, V = 1360 Å^3. Its structure has been solved by single crystal data, RI = 0.065, and also shows a layered framework. The structure solution procedures, the frameworks and the thermal decomposition products will be discussed.

Keywords: RIETVELD REFINEMENT AB INITIO STRUCTURE DETERMINATION PHOSPHONATES

CRYSTALLOGRAPHIC STUDY ON THE INCOMMENSURATE PHASE OF QUARTZ BY SR

K. Ohsumi[1] Y. Miyata[2] K. Hagiya[3] M. Ohmasa[3]
[1]High Energy Accelerator Research Organization (KEK) Institute of Materials Structure Science 1-1, Oho TSUKUBA IBARAKI 305-0801 JAPAN [2]The Graduate University for Advanced Studies, Department of Materials Structure Science [3]Himeji Institute of Technology, Department of Life Science

Introduction: Incommensurate phases have been found in many types of inorganic compounds, i.e. oxides, sulfides and so on, and most of their structures were analyzed as modulated structures in the higher order dimensions. Though quartz was found to be imcommensurate in narrow temperature range just below its transition temperature between low- and high form in early eighties, the structure has not been determined. For analyses of this structure and its structural phase transition, we obtained the diffraction data at more than fifteen temperatures below the transition point. Some results of the experiment are described below.
Experimental: Diffraction experiment was carried out using polychromatic synchrotron radiation from a bending magnet at the beamline 4B1 of the Photon Factory, KEK. The sample was once heated up in the high temperature region by using high temperature furnace attached to the diffraction equipment. Then Laue patterns of quartz was obtained by one hour exposure at every 0.1 K from upper limit of the low-quartz region to transition temperature.
Result: Diffuse streaks in three directions from main reflections appeared at first stage of raising temperature, and then satellite reflections were recognized in elongating diffuse streaks to be getting isolated. And gradually they disappeared up to just below the transition temperature. Substructure model of the incommensurate phase was assumed to be constituted with the averaged structure of two domains related with Dauphine twin, and examined in the three dimensional space based on 85 main Laue reflections. Refinement of this substructure is now successfully in progress.

Keywords: INCOMMENSURATE STRUCTURE' QUARTZ SYNCHROTRON RADIATION