PS21.01.21 N-DIMENSIONAL SPACE GROUP SYMMETRY ON THE WEB. A.Thiers, H.de Hilster, M.Ephraim, CAOS/CAMM Center, University of Nijmegen Toernooiveld 1 6525 ED Nijmegen The Netherlands

N-dimensional space groups play an important role in the description of incommensurate crystals, like quasi crystals and incommensurately modulated crystals. These types of materials can be looked upon as the intersection of the physical space with a higher-dimensional lattice periodic structure. The dimension of the latter is equal to the number of indices needed for the diffraction pattern.

The purpose of the programme is to provide information about the space groups of arbitrary dimensions. It allows for manipulation and inspection of the groups, e.g. subgroups, Wyckoff positions and systematic extinctions. Visualization of space groups, e.g. of the general or special positions or the space group elements, is done using VRML (Virtual Reality Modelling Language).

The number of space groups increases rapidly when one goes to higher dimensions. This makes it not feasible to present the information as a printed volume. The information, generated from data (generating elements) in a data base, or from user supplied data comprises the space groups, the symmetry elements, the Wyckoff positions and the general and special extinctions. The goal is to show all data present in the existing tables for 2 and 3 dimensions, with the benefit of choosing an arbitrary origin and setting.

The user computer interaction is realized using FORMs and POSTs sent between a special HTTP daemon and the user's WWW browser, giving the interactive feel of a local computer programme. The FORM interface features buttons of all kinds, input fields, checkboxes and selection menus.

PS21.01.22 ALGORITHM FOR CONSTRUCTION DATA BANKS OF THE CRYSTAL STRUCTURES WITH THE GIVEN CHEMICAL FORMULAS. V.R.Khachaturov, Computing Center RAS, Moscov R.V.Galiulin, Institute of Crystallography, Moscow

The Crystallochemical Shubnikov's law on coefficients ratio in chemical formulas according to multiplicity of thier Wyckoff positions in space group, creates the opportunity to enumerate all topologically different crystal structures for any set of chemical elements. The optimization of these types by packing with the account of ionic radii of their atoms, gives all metric realisations.

Each space group has special spectrum of multiplicity appropriate to it Wyckoff positions. For example, multiplicity spectrum of Wyckoff positions a,b,c,d,e,f,g,h,i,j,k,l,m,n in space group Pm3m is following: 1,1,3,3,6,6,8,12,12,12,24,24, 24,48. If the ratio of coefficients in crystallochemical formula is 1:1:3 (that takes place in perovskite) then atoms can take only five different sets of Wyckoff positions: a,b,c; a,b,d; g,g,k; g,g,l; g,g,m. To this cases correspond 3 topological different structures (positions c and d also positions l and m geometrically not distinguish). The last two types is not known. In case of chemical formula the number of different topological types for a given ratio infinitely, since it can be realise by the set of any Wyckoff position with free parameters. But use of Khacaturov's ray-method (Preprint of Computing Center Russian Ac.Sci., Moscow,1987, 26 p.) in the combination with the Vernadsky law on everywheresity of chemical elements permits to allocate the convex area in the space of chemical formulas with final number of integer points (polyhedron of chemical formulas), that has allowed work out this algorithm.

Topology II - Critical Points

MS21.02.01 CRITICAL POINT ANALYSIS IN PROTEIN DENSITY MAP INTERPRETATION. Suzanne Fortier[*][&], Antony Chiverton[*] and Janice Glasgow[&]. [*]Depts. of Chemistry and [&]Computing and Information Science, Queen's University, Kingston, Canada, K7L 3N6, and Laurence Leherte, Facultés Universitaires Notre-Dame de la Paix, Namur, Belgium

Critical point analysis has been investigated as a method to assist in the interpretation of protein electron density maps, as part of a project in molecular scene analysis. In particular, the usefulness of the topological approach for the segmentation of medium resolution (3Å) maps of proteins and their interpretation in terms of structural motifs has been assessed. Using the program ORCRIT (1), we have analysed the topology of calculated and experimental electron density maps through the location, identification and linkage of their critical points. The study has shown that critical point mapping can serve as a segmentation and pattern recognition tool in medium resolution maps of protein and that, in particular, it can be used for tracing the main chain of the protein and identifying secondary structure motifs. Furthermore, it was observed that at 3Å resolution, each residue in the polypeptide chains is, in general, associated with only one peak in the main branch of the critical point networks. Thus the approach allows for the parsing of the electron density maps into super atoms corresponding to the residues. The critical point method is now being combined with the treading approach, commonly used in protein structure prediction work, to help align sequence onto structure.

1. Johnson, C.K. (1976). ORCRIT. The Oak Ridge Critical Point Network Program. Chemistry Division, Oak Ridge National Laboratory, USA.

MS21.02.02 THE MEASUREMENT AND USE OF TOPOLOGICAL FEATURES OF THE EXPERIMENTAL ELECTRON DENSITY V.G.Tsirelson, Mendeleev University of Chemical Technology, Moscow, Russia

The quantum topological theory, developed by Bader, allows to analyze the chemical bond, intermolecular interactions and properties of molecules and crystals in terms of the features of the electron density which can be measured experimentally. The experimental electron density, however, is dynamic and suffers from both statistical uncertainty of the measurement results and Fourier series truncation error. When the multipole modelling of the electron density is used, the model error can be significant as well. All these circumstances influence the topological characteristics obtained.

There are three methods of calculation of the topological features of the experimental electron density. One of them is based on finite-difference calculation of the derivatives of the electron density presented in the Fourier series form. The second method uses combination of promolecule and deformation electron densities. The third method is based on model description of the electron density. The advantages and shortages of each of these approaches are discussed in this talk. The results of the experimental topological studies of inorganic, organic and organo-element compounds show that semi-quantitative agreement with theoretical data is observed as a rule.

The use of topological features of the experimental electron density for study of non-standard cases of the chemical bond, long-range interactions in solids as well as for the ground of some crystal chemical notions are discussed.