PS22.02.08 DIAMOND - A VISUAL CRYSTAL STRUCTURE INFORMATION SYSTEM by K.Brandenburg, University of Bonn, Germany

Scientists, interested in crystal structures, want to handle crystal structure information independent of their origin. A general system should therefore manage information from all sources: CRYSTMET, CSD, ICSD, PDB as well as CIF's and SHELX files from the crystallographers own laboratory.
Retrieval should be possible for all kinds of queries: chemical and structural, mineralogical and technical, symmetry and bibliography relevant questions.
The system should support all further investigations based on structural information: calculation of atomic distances, statistical evaluation, relations between structures, estimation of physical properties, etc. Last but not least an informative threedimensional representation of any structure should be available and results should be transferable to any other medium.

All these features should be possible without tricky commands in modern menue technique with window and point-and-click functions. DIAMOND is designed to fulfill all these conditions. Up to now the basic functions are available with special accent on the visualization of structures. Wireframe, ball-and-stick, space-filling and polyhedra models are supported. Infinite lattices can be built up step by step by adding spheres around initial atoms. Molecular fragments are found and completed automatically without explicit given connectivity. Surfaces in any direction can be represented. Atoms can be selected in any size and color, with and without thermal ellipsoids.

The power of the system will be demonstrated by several pictures. You are invited to bring your own files to the booth and to test the system immediately.
Further information can be obtained from WWW: http// www.rhrz.uni-bonn.de/~unc442/diamond.html

PS22.02.09 CRYSTAL CHEMICAL RESEARCH POTEN-TIALS OF DATABASE ON PROPERTIES OF MATERIALS FOR ELECTRONICS. S.A. Magarill, S.V. Borisov, N.V. Podberezskaya, L.M. Volkova, Institute of Inorganic Chemistry Sib. Branch RAS, Novosibirsk, Russia, Institute of Chemistry FE Branch RAS, Vladivostok, Russia

Using the data of the 'Crystal Structure' section of DB PME [Zh. Strukt. Khim. (Rus.), 1995, v.36, N3, p.559-562] as the base, we have carried out a crystal chemical analysis of some high-temperature superconducting compounds, considered accumulation and transfer of charges in superconducting cuprates, predicted new copper-free high-temperature superconductors, and published reference books involving reviews, data and bibliography. Crystal chemical calculations were performed and correlations were found for crystal structures of copper-containing phases, copper-free oxides superconductors, oxide bronzes, and rare-earth chalcogenides.

A structural similarity between various compounds was revealed by using planar atomic nets. These allowed us to compare structures, separate the planes with a densest atomic filling, and estimate a possible heteroepitaxy, i.e. to predict a possibility of the epitaxial growth of a target material on the substrate oriented in a certain way.

The structures of inorganic coordination compounds were considered as the packing of the quasi-spheres of the R_{ef} radius which form cubic (CaF_2 and $NaCl$ or combinations thereof) or hexagonal structure types. The R_{ef} radius of the basic sphere was applied to estimate the lattice parameters of the hexagonal ($a_h=2R_{ef}$) and cubic ($a_c=22 R_{ef}$) unit cells. The estimated lattice parameters

are comparable with the observed ones. This suggests a possibility for co-crystallization and the isomorphous substitution. We observed a successive conversion from the cubic to triclinic symmetry with preserving packing rules of the complex centers as the most 'hard' scattering fragments.

These results can be used as the elements of the chemical design required for an aimed synthesis of crystals with specified properties.

*Magarill S.A., Borisov S.V., Podberezskaya N.V. et al //(Zh. Struct. Khim., 1995, v.36, N3, p.559-562).

PS22.02.10 AN IDENTIFICATION SYSTEM USING CHEMICAL INFORMATION IN MODIFIED EXISTING DATABASES. A.R. Hölzel, Systematik in der Mineralogie D-55270 Ober-Ölm, Ulmenring 11, Germany

A computer program package is developed to identify inorganic phases or metal organic complexes using quantitative chemical analysis data. Crystal-chemical terms allow the search for variable compositions within solid solution series or related compounds. The use in combination with other parameters, e.g. X-ray, crystal-data, etc. is possible.

The database contains the chemical composition and crystal-chemical terms by weight- and atom-%, mostly derived from the sum formula using existing databases. The grouping of the crystal-chemical terms is based on:
1. The periodical table of the elements, Group 1Aa to 8Bb - H,(D,T) to Platin Group Elements with subdivisions depending on chemical behavior or ionic radii, e.g. group 1A splits into 1Aa=H,D, and T; 1Ab=Li; 1Ac=Na to Fr,
2. Three additional Groups, containing only micro- probe detectable elements, here defined by Na and all elements of higher atomic weight. <L> to the large and <M> to the medium to small cation radii elements. <E> collects all micro-probe detectable elements. These group symbols will be handled like element symbols.

E.g. a description by wt.-% of a compound like $NaAl[SO_4]_2*12H_2O$: Na—5.02 Al—5.89 S-13.98O-69.84 H—5.28 1Ac—5.02 3Ab—5.89 6Ab-13.981Aa—5.28 6Aa-69.84 L—5.02 M—5.89 E-24.89.

A search using analysis data with intervals will find this compound, a similar search with atom-% will find the whole family.