KY.NT.01 MULTIWAVELENGTH ANOMALOUS DIFFRACTION (MAD) IN MACROMOLECULAR STRUCTURE DETERMINATION Wayne A. Hendrickson, Howard Hughes Medical Institute, Department of Biochemistry and Molecular Biophysics, Columbia University, New York, NY 10032 USA.

There has been a recent explosion in the determination of protein and nucleic-acid crystal structures from multiwavelength anomalous diffraction (MAD) data. The possibility of evaluating phases from MAD measurements has been appreciated since the 1950's, and practical implementations of the method were demonstrated over ten years ego. Nevertheless, maturation into a routinely applied method has been somewhat slow in coming. Major contributors to the recent successes include increased availability of appropriate synchrotron beamlines, cryopreservation so that one crystal can suffice for a complete analysis, general methods for incorporating anomalous centers as in selenomethionyl proteins and brominated nucleic-acid basis, and increasingly sophisticated computer programs for data analysis. Recent applications, potentially complicating problems, and future prospects will be discussed.

KY.NT.02 NOVEL CRYSTAL PHYSICS UNDER PRESSURE. Y. Fujii, Institute for Solid State Physics, The University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan

Application of pressure to a crystal provides a unique opportunity to study interatomic interactions controlling its crystal-, magnetic-, and electronic-structures. A crystal lattice shrunk by pressure causes a significant change in these interactions resulting in phase transitions through reconfiguration of electrons, atoms, and molecules. By following a brief overview of the state-of-the-art in "high pressure crystallography" highlighted in six consecutive Microsymposia, we present several novel crystal- and magnetic-phases stabilized under pressure which have been investigated structurally and dynamically by x-ray and neutron scattering techniques: (1) Superconducting Metallic Halogens - A molecular-to-monatomic transition preceeded by the gradual metallization takes place in elemental diatomic molecules I_2(21GPa), Br_2(80GPa), and IBr(39GPa). A scaling rule with respect to their crystal lattices holds upon metallization, resulting from electron delocalization process directly observable by a MEM method using reliable intensity data. Also observed in iodine are further successive phase transitions in its monatomic superconducting phase, ultimately leading to an fcc lattice stabilized above 55GPa. Pressure collapses molecules and creates exotic materials. [H. Fujihisa et al., J. Phys. Chem. Solids 56, 1439 (1995).] (2) Devil's Flower- Dielectric compounds, $[N(CH_3)_4]_2MC_{l4}$ (M=Zn,Fe,Mn) having frustrating inter-radical interactions, display a large number of high-order commensurate phases intervening in nominally incommensurate phase in its P-T phase diagram in shape of an infinite number of petals. Also observed is a universal phase diagram for these compounds. Pressure controls a delicate balance of interactions. [S. Shimomura et al., Submitted to Phys. Rev. B.] (3) Spin-Peierls System - An inorganic spin-Peierls compound $CuGeO_3$ with a one-dimensional chain of S=1/2 spins on Cu displays a remarkable pressure effect on its dimerized lattice and spin-gap resulting from a singlet ground state below 14K at atmospheric pressure. Pressure controls a system dimensionality. [M. Nishi et al., Phys. Rev. B52, 6959 (1995).]

KY.NT.03 PREFERENCES AND EXCEPTIONS IN ORGANIC CRYSTAL PACKING MODES Vitaly K. Belsky, L. Karpov Institute of Physical Chemistry, Moscow, 103064, Russia.

1. A glimpse at the problems history (Kitaygorodsky's theory of close packing, earlier attempts to systemize the organic crystals data).
2. The concept of structural class (SC) as a unity of crystals of the same space group and the same list of systems of equivalent positions (orbits), occupied by molecules - base for statistical treatment of organic homomolecular crystals.
3. The analysis of the distributions by SC, categories, space groups, chiral types etc.
4. The elite and monstrous modes of organic molecules packing.
5. Multisystem crystals and supersymmetry.
6. Tendencies in distributions data.
7. Molecular own symmetry, pseudosymmetry and orbits symmetry (symmetry of position).
8. What is all this for?

KY.NT.04 RELIABILITY OF PROTEIN STRUCTURE DETERMINATION. T. Alwyn Jones & Gerard J. Kleywegt. Department of Molecular Biology, Uppsala University, Biomedical Centre, Box 590, S-751 24 Uppsala, Sweden

The reliability of protein structure determination depends on many factors, not least of which is the experience of the crystallographers involved. The kinds of errors introduced into a model during the initial map interpretation will be discussed. The identification of these errors requires a refinement protocol that is suited to each study. Different protocols depend primarily on the resolution of the study, and the number of NCS copies in the asymmetric unit. A policy of constant model evaluation during the refinement process is needed in all protocols. We suggest that the community can do a better job of refining macromolecular structures. Whether the community actually does a better job, seems to depend on the policy controlling the deposition of structure factor data.

KY.NT.05 STRUCTURES OF SURFACES STUDIED BY X-RAY DIFFRACTION. Robert Feidenhans'l, Department of Solid State Physics, DK-4000 Roskilde, Denmark

In surface science the use of x-ray scattering has developed to the point where it now can be applied to solve a great diversity of problems, including complex reconstructions, surfaces in electrochemical cells, solid/liquid interfaces and much more. These developments have relied both on improvements in sources of synchrotron radiation, and on our understanding of how to exploit them for the study of surfaces.

After an historical overview, the basic principles of the technique will be discussed. Examples of complex reconstructions of surfaces induced by adsorbates (sulphur on metal surfaces and surface alloying) will be shown, where the structures were solved using methods adapted from conventional crystallography. The talk will conclude by comparing x-ray scattering with other surface structural tools and discuss future directions using examples of surface science performed under non-ultra-high vacuum conditions.