

data have been used. At least 3-4 computer programs handle multi-phase refinement. In zeolite ZSM-5, 180 parameters were refined from x-ray data (Baerlocher). Applications to polymers have been made effective by use of constrained-molecule refinements (e.g. Pawley; Immirzi). A particularly fruitful new development is the use of the Rietveld method with intense pulsed neutron (time of flight) data, used for most of the >50 powder diffraction studies reported from the IPNS-Argonne from 1981 on. Precision in atomic parameters comparable to good single crystal results is usual with non-hydrogenous materials.

Some developmental needs outstanding for Rietveld analyses are better modeling of reflection profile shapes, better handling of preferred orientation, how to recognize and avoid false minima, improvement of techniques and methods so that good individual temperature factors can be routinely determined simultaneously with site occupancy factors, resolution of the current discussions of standard deviations, and an equivalent of the Hamilton R-ratio test.

Appropriate modeling of the reflection profiles can be crucial to several types of analyses. Further progress has been made on the problem, both by use of simpler geometries (HDS) and with improved models.

Recent progress in line profile analysis includes advances in single-line analyses, incorporation of size and strain parameters in a Rietveld refinement program, and very sophisticated analyses to determine the detailed nature of disorders in lamellar structures (e.g. Tchoubar, et al.)

Progress in the phase identification and quantitative analysis is being enhanced by improved precision of data, pattern decomposition, and instrumental resolution.

**ML.12-H4. FUNCTIONAL SIGNIFICANCE OF FLEXIBILITY IN PROTEINS.** By Robert Huber and William Bennett, Max-Planck-Institut für Biochemie, 8033 Martinsried/München, FRG.

The structural basis and the functional implications of large-scale flexibility are discussed for three systems: trypsin-trypsinogen, immunoglobulins, and citrate synthase. The trypsin-trypsinogen system provides an example in which an order-disorder transition is used as a means to regulate enzymatic activity. Immunoglobulins demonstrate how flexibly linked domains may be used to allow the binding of ligands with diverse arrangements. In citrate synthase, domain motion forms an active site that is shielded from solvent. Analogous large-scale flexibility has been observed in a number of other systems.

**ML.13-H2 CRYSTALLOGRAPHIC CONCEPTS IN THE DESIGN OF MATERIALS FOR THE DISPOSAL OF NUCLEAR WASTE.** By F.P. Glasser, Department of Chemistry, University of Aberdeen, Old Aberdeen AB9 2UE, Scotland.

Radioactive wastes must be immobilized in a form which effectively isolates them from re-entering the biosphere for long periods of time, ranging up to  $10^5$  -  $10^6$  years. The species requiring immobilization lie mainly in the atomic number range 40 - 72, together with Th, U and other actinides. Geological barriers may be insufficient for their containment, especially for those having high geochemical mobility. Matrix isolation, siting individual atoms in dilute solid solution in the lattice of a crystalline phase or phases, can be used to design high-integrity waste forms. The waste form is typically achieved by balancing the waste composition with oxide additives, tailored to achieve the desired phase combination after a ceramic fabrication and firing stage. The principles of crystallochemistry and phase equilibria are used to design satisfactory phase combinations. Examples are presented showing how these principles have been applied. Special applications arise for crystalline host phases which are suited to the immobilization of normally gaseous elements, e.g. tritium. Degradation of crystalline host lattices may occur by leaching, accelerated by lattice damage arising from radiation, transmutation, fission product accumulation, etc. These effects are discussed. The science of developing high-integrity materials which are durable in a wide range of natural environments is in its infancy. However, the fruits of decades of crystallochemical and phase equilibria research have enabled remarkable progress to be made, thereby offering hope that radioactive wastes can be effectively immobilized by a combination of man-made and natural barriers.

**ML.13-H4 MEASUREMENT AND USE OF ANOMALOUS X-RAY SCATTERING.** By Wayne A. Hendrickson, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D. C. 20375, U.S.A.

X-ray scattering factors are affected by resonance of the incident radiation with natural frequencies of bound electrons in atoms. This anomalous scattering grows very large as the absorption edges of certain ionic species are approached, but it is also substantial at wavelengths remote from edges. In practical terms, for all but the lightest of atoms, anomalous scattering is the norm at wavelengths of interest for diffraction experiments. Appropriately designed experiments can isolate the contributions of a few anomalous scattering centers from among many normal scattering light atoms. The distinctiveness of these centers and the accompanying phase shifts make anomalous scattering useful in structure determination -- particularly so in macromolecular crystallography. Phase information from anomalous scattering measured at a single wavelength is inherently ambiguous and must be combined with other information to be definitive. The combination with isomorphous replacement results is standard. Recent advances have been made in methodology for using partial structures, solvent leveling, and direct methods to resolve this phase ambiguity. In addition, it has long been recognized that, in principle, multiple wavelength analyses can yield definitive solutions. Measurement and processing techniques to eliminate systematic errors are essential for anomalous scattering data. But although small, the effects can be powerful. For example, the actual signal in Bijvoet differences arising from the sulfur anomalous scattering ( $\Delta f''=0.6e$  at  $\lambda=1.54\text{\AA}$ ) of the protein crambin averaged only 2.1% of  $|F_{\text{obs}}|$ , yet this sufficed for a direct determination of the structure. Resolved anomalous phasing procedures have subsequently been used in other structure determinations. Several laboratories are engaged in synchrotron experiments to exploit anomalous dispersion at multiple wavelengths.