

**ML.18-A** X-RAY STRUCTURAL STUDIES OF ICOSAHEDRAL VIRUSES. By Michael G. Rossmann, Department of Biological Sciences, Purdue University, W. Lafayette, Indiana 47907, USA.

A few structures of both plant and animal viruses have been determined in the last few years. The highest resolution results on intact viruses are those of tomato bushy stunt virus (TBSV; Harrison et al., *Nature*, 276, 368-375, 1978) and southern bean mosaic virus (SBMV; Abad-Zapatero et al., *Nature*, 286, 55-59, 1980), both RNA-containing plant viruses. Studies of animal viruses have been more difficult, although D. Wiley and I. Wilson (unpublished) have been able to determine the structure of the hemagglutinin spike of influenza virus.

The major technological advances which have made it possible to determine structures with molecular weights in the range of 2 to  $10 \times 10^6$  have been:

1. commercially available and reliable rotating anode generators, now being augmented by synchrotron sources, to generate high intensity X-rays;
2. fine-focusing X-ray sources and focusing mirrors to obtain the necessary resolution of Bragg maxima for very large unit cells;
3. the development of oscillation photography in conjunction with fast film scanners to measure hundreds of thousands of reflections while the crystal is rapidly decaying due to radiation damage; and
4. the molecular replacement method which utilizes the non-crystallographic symmetry of viruses to help in the determination of heavy atom positions and to greatly improve the accuracy of phase determination.

Both TBSV and SBMV have an external diameter of around 300 Å and a protein coat of 50 Å or more thickness. Their interior is filled with RNA. The 180 protein subunits per virus have icosahedral symmetry. Although the viruses are quite different in many of their properties, the polypeptide topologies of their surface domains are remarkably similar. TBSV possesses an additional protruding domain. Investigation of other viruses such as satellite tobacco necrosis virus (Unge et al., *Nature*, 285, 375-377, 1980) will help to show whether this remarkable similarity is the result of divergence from a primordial plant virus or of constraints required for self-assembly into an icosahedral particle.

The basic amino terminal arm of SBMV, TBSV and many other spherical and bacillus-shaped plant viruses is intimately involved in RNA interaction and the assembly of the protein subunits into a coat of appropriate diameter. The surface domain of SBMV is an eight-stranded anti-parallel β-barrel. Protein-protein interactions are mediated by the binding of cations and hydrophobic interactions. Removal of calcium causes the virus to swell and then disassemble. Protein-nucleic acid interactions are also enhanced by a basic surface on the interior of the surface domain.

**ML.18-B** QUANTITATIVE ASPECTS OF SYSTEMATIC CRYSTAL CHEMISTRY. By W.B. Pearson, Faculty of Science, University of Waterloo, Waterloo, Ontario, Canada.

A review of the contents of the various volumes of *Acta Crystallographica* reveals that the solution of crystal structures and the applications of mathematical analysis, are the continuing major interest of crystallographers. To a much lesser extent, but with no less elegance, there is an interest in the descriptions and interrelations of crystal structure types according to symmetry and connectivity principles. On the other hand, interest in accounting quantitatively for the physical properties of compounds or phases on the basis of the structural arrangements of the atoms is almost nonexistent. Perhaps some of the excitement of this field, in which so much work is to be done, can be transmitted, by showing how previous hindrances to progress - such as coordination number - can be avoided. Also to be avoided is examining properties in terms of the radius ratio which hinders interpretation, because of the intractable nature of ratios. Another hindrance, particularly in alloys, has been lack of knowledge whether the valency of an atom differs in its alloy from that in its elemental structure. Such differences can now be detected and interpreted, generally on a quantitative basis.

If the new methods of analysis have so far applied to unit cell dimensions, it is because this is by far the largest data set of physical properties that we possess, but there is no reason why they should not be applied to any set of physical properties. The analysis of cell dimensions leads first to identification of the atomic arrays that control them (a fact which may be by no means obvious in a complex structure) and thence entirely new information concerning structural properties may become apparent. Time will limit the discussion largely to metals and alloys, but it is hoped that attention can also be drawn to developments involving inorganic structures.

**ML.19-A** SYNCHROTRON RADIATION AND ANOMALOUS DISPERSION. By H.B. Stuhmann, EMBL-Outstation Hamburg, Notkestrasse 85, 2000 Hamburg 52 / Germany.

The method of phasing Bragg reflections by anomalous dispersion using synchrotron radiation (Phillips, Goodfellow, Watenpugh, Sieker, Jensen & Hodgson, *Acta Cryst.* (1977) A33 445-455) is extended to the study of semi-crystalline structures, amorphous material (Fuess, SSRL Report 80/06) and solutions (Stuhmann, *Acta Cryst.* (1980) A36 996-1001). The anomalous scattering factors are only a fraction of the scattering length of heavy atoms (Templeton, Templeton, Phillips & Hodgson, *Acta Cryst.* (1980) A36 436-442). However, the measurement of anomalous scattering effects can be reasonably precise, as reduction and scaling of data is facilitated by the dispersion law known from the X-ray absorption spectrum. The use of position sensitive area counters is a particular advantage. That the accuracy of the intensity measurement of 0.001 is needed in macromolecular structure investigation by anomalous dispersion and that it can be achieved has been shown recently in the case of dissolved hemoglobin (Stuhmann, submitted to *Proc.Nat.Acad.Sci.*, USA).

Anomalous scattering is also a promising tool in membrane structure research, as is apparent from investigations going on at SSRL (Stanford, USA) and EMBL (Hamburg, Germany). It also may have an impact on fibre diffraction.