

# In this issue

## Michael G. Rossmann, friend of India

The structure of canine, parvovirus, determined recently by Rossmann's group is reported in the 'Research news' column of this issue (page 620). This is the first example of an isometric DNA virus whose three-dimensional structure has been determined by X-ray diffraction techniques. However, this is only one of the 'firsts' of Rossmann's achievements. Rossmann has passionately pursued development of techniques for the determination of increasingly complex structures of biological macromolecules and methods of eliciting functional and evolutionary information from structures. It has been a great privilege to know Rossmann for the past three decades. He is a *great friend* of Indian crystallography.

Michael G. Rossmann, Hanley distinguished professor of biological sciences, member of the National Academy of Sciences (USA), leads a large team of X-ray crystallographers and structural biologists at Purdue University, USA. Professor Rossmann is a world leader in macromolecular crystallography. Rossmann authored a classic paper, with D. M. Blow in the early sixties when he was at Cambridge University, which showed for the first time how symmetry properties of biological macromolecules can be deduced from X-ray diffraction data of their crystals. The isomorphous replacement technique, developed by Green, Ingram and Perutz, is the method of choice for the determination of protein structures. However, application of this method for super-large biomolecules such as symmetrical virus particles would have been intractable but for the automated 'vector search' methods developed by Rossmann's group. Rossmann has also contributed to the theoretical aspects of phase calculation and refinement and other aspects such as correlating the reference origin in different heavy-atom derivatives used in isomorphous replacement. Screenless oscillation photography was developed in the mid-seventies by Arndt and Wonacott as the method of choice for efficiently recording virtually millions of

reflections arising from crystals of large biological macromolecules. Rossmann has developed one of the most successful and intelligent computer program packages for processing these films. The electron-density maps obtained for very complex biomolecules and molecular assemblies such as viruses by the isomorphous replacement technique are often noisy and do not allow easy extraction of an image of the desired molecule. Again Rossmann's group has pioneered the development of the 'molecular replacement' techniques, which are powerful methods for reducing the errors in phases by imposing symmetry constraints on the initial, noisy map.

Rossmann's laboratory has enriched biological crystallography by offering a steady flow of newly determined structures of increasing complexity. Each molecule determined by his group was one of the largest of its kind during the initiation of the respective project. In the late sixties and early seventies, the molecules were dehydrogenases. These were followed in the seventies by structures of catalase, phosphoglucosyltransferase and southern bean mosaic virus. In the eighties, Rossmann's group has been remarkably active in elucidating the structures of several isometric viruses: variants of human rhinovirus, mengo virus and now canine parvovirus.

Apart from contributions to experimental and theoretical crystallography, Rossmann has made invaluable contributions to the problems related to protein folding and evolution. Soon after the structures of dehydrogenases were determined, Rossmann realized that the three-dimensional structures of proteins are conserved during evolution to a far greater extent than either the amino-acid sequence or their function. His group has developed rigorous, quantitative methods for the comparison of polypeptide folds leading to information on protein evolution and speciation. In recognition of his pioneering contributions to protein folding, a frequently encountered motif of protein structure, consisting of two parallel  $\beta$ -strands separated by an  $\alpha$ -helix, has been called the 'Rossmann fold'.

There is hardly any area of macro-

molecular crystallography that has not been profoundly influenced by Rossmann's work.

## Electricity in the air

Three geophysical electrical systems are known to exist: one in the atmosphere; the second within the earth due to currents flowing parallel to the surface; and the third which transfers electrical charge continuously between the atmosphere and the earth. A. K. Kamra discusses (page 639) how human activity can interfere with and modify these electrical processes. There are a multitude of ways by which this can occur. Deforestation, desertification and even agricultural operations can introduce large amounts of dust into the system, causing dust storms. A serious study of cities in the USA (project Metromex) indicates that changes in turbulence and albedo due to urbanization can affect cloud coverage and rainfall patterns. Air pollution due to industrial activity especially in the Northern Hemisphere, exhaust fumes, etc. would decrease the atmospheric electrical conductivity which may possibly be compensated for by the radioactive krypton-85 released from many nuclear energy stations. Even low-frequency transmitters and power lines can alter the telluric currents in the earth. The work done in India in this field is also reviewed. Electrical changes can, in theory, affect the dynamics of water-drop coalescence in clouds, which may affect weather and climate. What seems difficult is to get quantitative estimates of many of these effects as also to assess their relative importance.

## More energy from waste?

To get energy from waste is the order of the day. M. Srinivasan and co-authors suggest (page 647) a very novel method of deriving energy from nuclear waste, killing two birds with one stone! A nuclear reactor during its operation produces isotopes of actinide elements, which are radioactive, with long half-lives. These radioactive wastes have to

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be disposed off by treatment along with fission products. To remind ourselves, natural uranium contains less than one per cent uranium-235, the rest being uranium-238. Uranium-235 is the fissile material used (after enrichment to 3%) as fuel in most nuclear reactors. Uranium-238 is not wasted, for when it absorbs neutrons in a nuclear reactor it too becomes 'fissile', and is used for generating power. Another such isotope, uranium-233, is produced by thorium-232 absorbing neutrons. The actinides referred to earlier do not belong to these two classes but are considered useless, with a nuisance value presenting serious problems of waste disposal. Srinivasan and co-authors suggest that, although these actinides cannot sustain a chain reaction in a nuclear reactor with thermal neutrons, they are 'fissible' because they can sustain a chain reaction with fast neutrons. They are therefore potentially valuable nuclear-fuel materials and not waste. The authors report their systematic studies of the criticality parameters of these 'fissible' isotopes.

### Dating mantle-derived rock

Carbonatites are magmatic rocks containing more than 50% by weight of carbonate material. While these were known to occur in Africa, Australia, North America and the Soviet Union, they were first observed in the Indian

subcontinent in 1963 in Gujarat in Amba Dongar (the 'hill of mangoes'). Carbonatites have since then been discovered in widely spaced localities in India, like Sevattur in Tamil Nadu. It is one of the intrusions which include those at Elagiri hills and Salem. A major problem that confronted geologists was whether these Cretaceous limestones were altered and mobilized by Deccan volcanism (65 million years ago). Most of these carbonatites contain magnetite, apatite and biotite. Anil Kumar and Gopalan have made (page 653) very precise age measurements using the Rb-Sr method. They arrive at a date of 771 million years to an accuracy of 2%. Geochronologists have to establish that contamination of the relevant element (in this case Sr) has not taken place after 'the event'. By careful studies the authors show that the carbonatites (and their constituents) and the magma have almost identical Sr-isotope composition, so that all indications are that the former crystallized from the latter and that there has been little contamination or post-magmatic alteration. However, the carbonatites of Sevattur have higher Sr isotopic ratios than those of Africa, Australia and North America, for which the authors attempt an explanation.

### Carbenes

Carbenes are known to be extremely

reactive, transient intermediates. S. S. Krishnamurthy tells us (page 619) of the exciting story of how these have recently been actually crystallized. No lack of miracles in chemistry!

### Greening the mind

M. S. Swaminathan seems to have an inordinate capacity to attract international prizes and awards. We reproduce (page 633) the lecture entitled 'environment and development' which he gave while accepting the Tyler prize for environmental achievement. In this he pleads for the 'greening' of the human mind so that the 'greening' of the earth can naturally follow. Gandhi said: 'How can we be non-violent to nature unless the spirit of non-violence becomes an ethos of human culture?'

### Effects of Gulf smoke

It is very gratifying to note that after detailed studies (calculations using their model), the India Meteorological Department predicted, as early as January/February 1991, that the oil fires in the Persian Gulf region will not have any perceptible effect on the Indian summer monsoon of 1991. This has now been verified in detail independently by the computer-modelling studies made by the Meteorological Office, London, and the Max Planck Institut für Meteorologie, Hamburg, Germany. See page 622.