

S. Ramaseshan: The crystallography phase

We were fortunate to be associated with S. Ramaseshan in the 1953 in the years when his attention had turned to the developing technique of X-ray crystallography. His early interest was in an experimental approach for solving the phase problem in centrosymmetric crystals. Together with his students, K. Venkatesan and N. V. Mani he showed that the intensity data collected using two appropriate wavelengths, close to the absorption edge of the atoms in the crystal, could be used to determine the signs of the X-ray reflections. The crystal structure of $KMnO_4$, in which the Mn atom was the anomalous scatterer was successfully determined. Following this he proposed a novel approach for determining the phase angles without ambiguity in non-centrosymmetric crystals. The method proposed used intensity data collected for two wavelengths on either side of the absorption edge of one of the atoms in the crystal. This idea, discussed as early as 1957 in a published paper, forms the basis of the Multiple Anomalous Dispersion (MAD) method now used extensively in solving the structures of protein molecules. During his stay at Oxford (1962–64) it struck him that the anomalous scattering of neutrons could be used to solve the phase problem for molecules with a large number of atoms; an idea he presented in a paper published in *Current Science* in 1965. His contributions to the development of anomalous scattering methods are indeed highly significant.

Ramaseshan built a group which rapidly contributed in various areas of crystallography. M. A. Viswamitra developed low temperature techniques to determine the structures of 'crystallized liquids', to study thermal expansion and transformation of crystals and to measure Debye–Waller temperature factors. S. Swaminathan and E. Misovic who came from Yugoslavia,

investigated planar polyaromatic structures. One of us (HM) was assigned the structure determination of the alkaloid, echitamine, whose constitution was being hotly debated by four groups of chemists in different countries. The structure determined by X-ray crystallography turned out to be different from that proposed on the basis of chemical evidence. The use of anomalous scattering from an iodide derivative permitted determination of the absolute configuration of the alkaloid. The group also studied inorganic compounds (N. V. Mani and Shivashankar Rao). The icosahedron, missing in Pauling's classical work, was identified as a coordination polyhedron in barium perchlorate.

The investigations in Ramaseshan's laboratory in the 1950s and early 1960s were mainly experimental, although the theoretical background was intensely discussed. Looking back, it is amazing that so much could be achieved with limited facilities. X-ray intensity data were collected using a single Weissenberg camera shared by about five students in the period 1953–59. There was tremendous understanding among the students, who shared a feeling of belonging to a single family – a crystallographic family. This in no small measure was due to Ramaseshan's charming qualities. The laboratory was run informally and lifelong friendships established. He was easy to work with, unhesitatingly generous and open to discussions. He encouraged students to do their best and develop their interests and ideas. He was intimately involved in their work, moving from desk to desk in the laboratory discussing progress and problems. An example of his intensity and passion for science immediately comes to mind. During the work on the anomalous dispersion method he would stay late in the laboratory at night and help the student in the laborious



calculations of Fourier summations and structure factor calculations using Beevers–Lifson strips.

Ramaseshan was a superb lecturer. The simplicity and directness of his physical intuition were remarkable. His contributions to the growth of crystallography in India is enormous and many of his students and their students occupy high positions in scientific institutions, making important research contributions. Recalling our association with Ramaseshan we must mention his wife Kausalya. If life in his laboratory was memorable for the students, it was in no small measure due to Kausalya Ramaseshan. Her devotion to her husband brings to one's mind what Sita was to Lord Rama, in the *Ramayana*; the epic which they loved to read and discuss. Rarely do we come across a scientist like Ramaseshan in whom the attributes of a great researcher coexist with the warm qualities of a wonderful human being.

K. VENKATESAN
H. MANOHAR*

*D-1, Himagiri Apartments,
77, 4th Main Road,
Malleswaram,
Bangalore 560 055, India
e-mail: kv@orgchem.iisc.ernet.in
*1, 9th Main Road,
Malleswaram,
Bangalore 560 003, India*