RAMACHANDRAN SRINIVASAN

(1933-2004)
Elected Fellow 1986

RAMACHANDRAN SRINIVASAN, a well-known crystallographer, passed away on 19th Sept 2004. He was associated with the department of Crystallography and Biophysics, University of Madras for the past four decades. Active crystallographic research flourished in the department under his leadership. His career in the University of Madras is almost synonymous with the growth of the Department of Crystallography and Biophysics. He was respected in the country and abroad for his contributions to crystallography.

EARLY EDUCATION AND PROFESSIONAL CAREER

He was born on 5th July 1933 at Nannilam in Tamilnadu to Mr. Ramachandra Iyer and Smt. Abhirami. He was the youngest in a family of four children. All his brothers were also Professors in the University of Madras, though their fields of specialization were different. His father was a Central Government employee and his mother was a homemaker. He finished his schooling from Ramakrishna Mission School, Chennai. His B.Sc. (Hon.)(1953) and M.Sc degrees (1954) were from the University of Madras. He secured the first rank in the M.Sc degree program and won a gold medal. After completing his M.Sc. with distinction he joined the Physics Department of University of Madras for a Ph.D. degree in X-ray Crystallography, under the guidance of Professor GN Ramachandran.

Srinivasan had the good fortune to be associated with G.N. Ramachandran during the exciting and productive period of theoretical crystallography and biophysics in India. The department was the center of intense activity in statistical crystallography and structure solution methods. Those were the days of Beever-Lipson strips and Hollerith machines, in sharp contrast to the ubiquitous computers and microprocessors of the present day. There were hardly a dozen members in the department including the students. The students formed a cohesive group under the able leadership of Professor GN Ramachandran.

Srinivasan completed his Ph.D. in 1958 and was appointed as a lecturer in the same department. In 1962 he visited the Cavendish Laboratory, University of Cambridge under Commonwealth Fellowship Program. Subsequently he became Reader in the year 1962, and a full Professor in 1964, one of the youngest Professors in the history of University of Madras. He became Senior Professor in the year 1972, a distinction that is given only to very few exceptional scientists. He was the Head of the Department of Crystallography and Biophysics from 1969 till his retirement in 1994, excepting for a brief period of one year. He was a visiting scientist at the Department of Biological Sciences, Purdue University in 1968 and he used this

opportunity to write his famous book on Fourier methods in crystallography (3), which was co-authored by Professor GN Ramachandran. He trained more than 16 Ph.D. students who occupy high positions all over the world.

SCIENTIFIC CONTRIBUTIONS

His research interests included Theoretical Crystallography, Polytypism, Structural Biophysics, Nuclear Magnetic Resonance, Gemology and Musicology. He has published over 200 papers in National and International Journals of repute. He has edited or written over nine books and monographs. Some of his contributions have become textbook material. He was a thorough physicist and his approach to problems was always based on his expertise in Physics, Statistics and Mathematics.

He had a deep knowledge of Fourier Transform theory and he used this knowledge to develop many new methods for recovering information (atomic sites) from imperfect electron density maps containing noise. His earlier work on the theory of structure analysis and intensity statistics was done in collaboration with Professor GN Ramachandran and Dr. S Parthasarathy. They developed special Patterson and Fourier syntheses for use in crystal structure analysis. Among these, the phase synthesis, α, β and γ' syntheses proposed by them were very popular with crystallographers. They showed that the phase angles have an overwhelming importance in revealing the structure and that the amplitudes play only a secondary role. New methods for extracting the entire structure when part of the structure is known were developed and tested thoroughly. In this context, the β synthesis proposed by them was shown to be superior to other methods in revealing new atoms as well as suppressing wrong atoms. His group proposed several weighting functions for the improvement of Fourier maps in the early stages of structure analysis. His work on phase synthesis, syntheses for partially known structures, combination of isomorphism and anomalous dispersion data for structure solution was very well received and extensively quoted. These results are summarized in the monograph entitled "*Fourier Methods in Crystallography*" published in 1970 by John Wiley and Sons.

He applied statistics extensively to solve crystallographic problems. There are two aspects of crystallography in which statistics plays a role, viz. intensity statistics and the application of probability methods for the solution of the phase problem. Srinivasan's contribution was mainly in the field of intensity statistics. Some of the useful results obtained by him include a test for centrosymmetry, derivation of probability distribution of structure factors from a pair of related crystals, etc. He used the term " pair of related crystals" to represent the true structure of the crystal and the trial or model structure with which structure amplitudes are calculated. Thus the theory developed for a "pair of related crystals" could also be applied to isomorphous protein crystals of the addition type with appropriate modifications. The probability distributions of the structure factors were subsequently used to predict the theoretical behavior of different types of normalized R indices. He also derived three different correlation coefficients of the structure factors of related crystals. One among these, viz. the sigma A coefficient, finds use in present day protein crystallography.

He developed statistical tests for the presence of centrosymmetry in crystals that obey Wilson distributions. The study was extended to crystals with pseudo symmetry and to

crystals that exhibit a degree of centrosymmetry. The probability distribution of Bijvoet differences, the statistical treatment of unobserved reflections in least squares refinement, and statistical tests for isomorphism in crystals are some of his other contributions to theoretical crystallography. He published about 80 papers in the area of crystallographic statistics and a monograph with his colleague S Parthasarathy, entitled "Some Statistical Applications in X-ray Crystallography". The book was so well received that a Russian translation of this book was published in 1977. He solved more than 50 crystal structures, though this was not the main thrust of his research. Most of these were done to test the theories proposed by him.

He has made significant contributions to the theory of anomalous dispersion. He was one of the early groups of scientists who worked out the application of anomalous scattering to solve the phase problem. He pointed out that the phases could be determined using multiple wavelength anomalous technique as well as single wavelength anomalous scattering. He suggested that the phenomenon of isomorphism could be simulated with a single crystal by making use of the anomalous dispersion effect. Long before the advent of synchrotron radiation sources he proposed an "essentially unique" solution to the phase problem using single wavelength anomalous dispersion technique through a "Tangent Formula". In this paper he showed that the phases could be determined within an error of 15 deg. in the case of small molecules. This idea is used extensively in macromolecular crystallography after the tunability of X-ray wavelength was made possible through a synchrotron source.

Srinivasan and Chacko were the first to give a formal representation of the electron density $\rho(r)$ corresponding to anomalous components. This function can be used in a reductionistic fashion for structure solution of macromolecules. This work lead to a review article on "Applications of X-ray anomalous scattering in structural studies" in Advances in Structural Research by Diffraction Methods (1972). This work is still a standard reference on various applications of anomalous dispersion to crystallographic problems.

In the later part of his career, he concentrated on Structural Biophysics. A large amount of protein structural data was available in the seventies and this prompted him to suggest new ways of retrieving information from these data. He realized that a new set of parameters different from those used in small molecule crystallography would be required for the extraction of information from these data. In this context he proposed several new methods for characterization of biopolymers. The earlier method proposed by Professor GN Ramachandran used two parameters, ϕ and φ, for characterizing a biopolymer. Srinivasan reduced this to one parameter and carried out extensive analysis of protein data based on this idea. He introduced a virtual bond concept for biopolymer characterization.

He showed that the virtual torsion angle θ involving $C^{\alpha}_{i-2} - C^{\alpha}_{i-1} - C^{\alpha}_{i} - C^{\alpha}_{i+1}$ can act as a single parameter for describing a chain fold. This representation helped in identifying a new helix, viz. the ε helix. Similarly, other torsion angles such as θ' (involving two bonds ($C_{i-1} - N \ldots C_{I} - N_{i-1}$) of successive peptide planes) were proposed by him for characterizing β turns. He also proposed a new method to represent the local helical axis with four consecutive C^{α} atoms, which enabled him to obtain the best experimental helical parameters and to quantify the helical distortions with ease.

He further introduced a generalized single parametric characterization of any given biopolymer. He treated a biopolymer as a quasi-rigid system and used rigid body mechanics to establish the relation between successive monomeric units through a single rotation- superposition angle (Φ_s). For this purpose he considered C^β, C^α and C' as a rigid group, and $C_{i-1}{}^\alpha$, N, C' and $C_i{}^\alpha$ as the second rigid group. Φ_s then relates one group to the other by superposition of centers of masses of the two groups, and a rotation about a single axis of rotation. If Φ_s is plotted as a function of residue number, it acts as a fingerprint of the folding characteristics. The successive vectors defining the axis of rotation-superposition yield an "axoid" for the polymer fold, which brings into view the finer features of folding. In this method, comparison of two homologous proteins reduces to a linear comparison of the single parameter Φ_s. However, Φ_s actually gives information about conformational homology rather than structural homology. Several proteins were analyzed using the above method and several novel features were reported. The interesting feature of the above method is its scope and its applicability to any biopolymer, as long as one is able to identify rigid units. In fact this methodology was applied to nucleic acids to characterize both RNA and DNA and to identify base sequence dependence in the structure.

Srinivasan developed a solid state NMR laboratory from scratch and constructed a wide line NMR spectrometer with the help of his students. His main contribution in this area was on line shape analysis using truncated moments, which finds use in motional studies in solid state NMR.

The accumulated data on small molecules and proteins have a wealth of information, which needs to be carefully analyzed. In this connection Srinivasan felt the need for a crystallographic data center in India. He was the Founder-Director of the National Information Center for Crystallography (NICRYS), funded by DST for almost a decade. This was the first of its kind in Asia and served the Crystallography community in India for a long time.

He was an expert committee member of several organisation like the Union Public Service Commission.University Grants Commission, Department of Science and Technology and the South India Textile Industries Research Corporation.

He organised 6 International conferences within a span of 30 years. His organisational abilities helped the department faculty and students to interact with more than 500 distinguished international scientists, which included several Nobel Laureates like Professors Linus Pauling, Sir Lawrence Bragg, Dorothy Hodgkin, M Wilkins, Severo Ochoa, Stanford Moore and others. In 1985, as one of the Conveners, he was responsible for the organisation of an International Workshop on Molecular Biosciences and Biotechnology on behalf of the Industrial House SPIC.

He has widely travelled. He made a lecture tour of USA and Australia in 1968. He attended several International Symposia and he was one of the two member delegation of the Government of India to the International Union of Crystallography Congress in Kyoto in 1972. He was one of the speakers in the International Meeting on Anomalous Scattering of X-rays, Neutron and Electrons in Madrid, Spain in 1974. He visited USSR, as one of two members selected under UGC Cultural Exchange Programme.

PERSONAL QUALITIES

He was interested in Musicology and the physics of stringed instruments. He organized a special seminar sponsored by Sangeeth Natak academy in 1981 and edited a volume to which he contributed research articles involving computer application to music.

Srinivasan was a good administrator and commanded respect from his colleagues and subordinates. He was a man of few words and never showed his emotions in public. He steered the research program of the department for more than two decades after Prof. GN Ramachandran left the University of Madras. The department was known world over as Srinivasan's department in the post GNR era. He maintained the eminence of the department and attracted large funding from various agencies.

He was a good teacher and had a tremendous memory. His presence during departmental seminars always made the discussions interesting and the students learned from these discussions. He served the crystallographic community by organizing several National and International seminars on Crystallography and Biophysics. More than 100 renowned foreign scientists from 10 different countries attended the International Seminar on Biophysics organized by him in 1978. He actively participated in the proceedings of the Madras Science Association. He also conducted monthly seminars under the aegis of the INSA Madras Chapter.

HONOURS AND AWARDS

He was an elected fellow of Indian Academy of Sciences (1968), Indian National Science Academy and Institute of Physics (London). He was a Founder Member of Tamil Nadu Academy of Sciences, and an executive- committee member of the IUCr. Teaching Commission, National Committee for Crystallography and the Indian Biophysical Society. He guided more than 16 research students.

He was an elected Fellow of New York Academy of Sciences and a member of the National Committee for CODATA. He was elected the President of Indian Biophysical Society in 1989.

LAST DAYS

After his retirement, he continued as INSA Senior Scientist in the same department. Two months before his demise, he participated in the making of the documentary film "The Immortal Coils " prepared by CSIR and Vigyan Prasar on his mentor Professor GN Ramachandran.

He was a visionary, was well ahead of his contemporaries. Till the end, he canvassed for a synchrotron source to be made available in India for macromolecular data collection, as well as to test his theories on anomalous dispersion method. He was interested in watching cricket and listening to music.

He was a devoted son and brother. He shouldered the responsibility of looking after his parents to a very old age; He looked after his brothers through their illness. He developed diabetic related complications in the last year, but he was cheerful till the end. His wife and

daughter survive him. His daughter Dhenuka, who is an environmental scientist, says, "My father was not only highly intelligent, but also modern and futuristic in his prolific ideas. He always believed in freedom of expression, independence and personal individuality" He leaves behind a host of students, colleagues and friends whose lives he enriched for the past four decades. All will cherish his memory and he will continue to inspire crystallographers the world over.

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