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Chemical crystallography in India

This is with reference to the article ‘Some themes in chemical crystallography pertinent to the Indian contribution’ by Desiraju¹. I was particularly interested in Section 1: ‘When did chemical crystallography start in India? Why did it not start earlier?’ Having been associated with the field since the late 50s, I wish to make the following observations.

As Desiraju mentions, crystallography in India began in physics departments, primarily because, in my view, chemists while interested in the structure, did not have the necessary mathematical background. In the early days crystal structure analysis was done manually using visually measured X-ray photographic data, with mathematical calculations including Fourier summations and least square refinements in two dimensions using an electrical calculator. I recall the time when chemists from the Organic and Inorganic Chemistry Departments at the Indian Institute of Science (IISc), Bangalore would come over to the Physics Department with their crystals for structure solution. In fact, for the structure determination of echitamine iodide, which was my Ph D problem, the crystals were sent to us from Madras (now Chennai) by the eminent organic chemist,

T. R. Govindachari, of Presidency College. The situation, however, changed in the late 70s with the advent of computer-controlled diffractometers, together with software packages for structure determination. With more accurate data and more computing power available, crystallographers could take up, apart from crystal structure analysis of larger molecules, more challenging problems like polymorphism, charge density studies, crystal engineering, etc.

Realizing the importance of this powerful analytical tool, the Inorganic and Physical Chemistry Department at IISc in a far-sighted move, decided to create a faculty position in the Department to train students of chemistry and initiate research in the field. I had the privilege of being selected for this position and joined the Department as a Lecturer in the summer of 1965. Thus, chemical crystallography had its ‘formal’ beginning in India in that year and not in the mid to late 70s as Desiraju concludes.

A home-made Weissenberg camera was constructed in the then Central Workshop and courses in crystal symmetry, X-ray crystallography and crystal structure analysis were delivered tailored to the needs of chemists. My early research

in the 60s and 70s was focused on the coordination chemistry of lanthanide complexes and conformational studies in cyclophosphazenes, both areas being investigated in the Department. Another line of research was the crystallographic aspects of solid state reactions. In the 80s, my research shifted to the synthesis and structural studies of metal interaction with molecules of biological interest. During the intervening period, inorganic chemists trained in X-ray crystallography had joined the faculty and started work in areas of their interest. All this goes to show that chemical crystallography in India had been initiated and practised successfully by inorganic chemists, rather than by physical organic chemists. As a footnote I may add that crystallography was introduced in the Organic Chemistry Department at IISc in 1971.

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