19-Crystallographic Teaching and the History of Crystallography

PS-19.01.09 SINGLE CRYSTAL X-RAY STRUCTURE ANALYSIS: THE DEVELOPMENT OF AN ANALYTICAL TECHNIQUE FROM THE INITIAL STEPS TAKEN BY KEPLER TO ITS APPLICATION IN CHEMICAL RESEARCH, ILLUSTRATED BY INTERNATIONAL POSTAGE STAMPS. By Hans Pruet, Fachbereich Chemie, Universität Dortmund, Postfach 50 05 00, D-4600 Dortmund 50, Germany.

"It is not often the case that the steps of the intellectual process are so clearly apparent as they are in crystallography." (200 Ans de Crystallographie en France, 10Cr Bordeaux 1990)


X-ray crystal structure analysis is an excellent example to demonstrate how different fields of science and technology contributed to form a complex analytical method. Postage stamps from all over the world will be used as a basis of a review of the method, its development from Johannes Kepler (1571-1630) to protein engineering, and some of the most important milestones in its history (Pruet, H. (1989). Chemie in unserer Zeit, 23, 101-129).

There are 16 magnetic point groups isomorphic with 4,2,2,2, which differ only in the way in which inversions are combined with proper rotation elements. The four scalars, e, e, τ, and η respectively transform by one-dimensional irreps g, g, g, and g, the first of which is identity, the remaining alternate. Since e transforms by g in g, 4,2,2,2, 4,2,2,2, 2,2,2,2, and 2,2,2,2, the tensor τ will transform in the same way and hence it will have the same equilibrium form as the tensor for u in these groups. The tensor τ will have this form in g, 4,2,2,2, 4,2,2,2, 4,2,2,2, and the tensor τ in g, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, and 4,2,2,2. The pseudoscalar e transforms by g in g, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, 4,2,2,2, and 4,2,2,2. The corresponding tensors have the same transformation properties and hence equilibrium forms in respective groups. Analogously we use the irreps g and g to apply to groups which contain some inversions explicitly.

This consideration has an interesting consequence. There exist only first possible nontrivial forms of tensors u, τ, τ, and τ in Lense class 4,2,2,2. Quite generally the number of possible forms equals to the number of real one-dimensional irreps of the group G, which is either one, two, or four.

The method is even more effective if taught together with Clebsch-Gordan multiplication which enables easy calculation of tensors. One table of transformation properties of tensors u under the group G together with a table of transformation properties of scalars under groups of Lense class G give then a transparent scheme which provides not only equilibrium tensors but also decomposition of tensors into bases of irreps. This relationship between tensors has been used recently (Gäbler, H. (1991). Acta Cryst. A47, 226-235), but the complete scheme has been described by the author a time ago (Koppély, V. (1979). Acta Cryst. A35, 83-95 and 95-101).

An elementary knowledge of representation theory is the price for this transparent approach which gives an insight into the system of mutual relations between tensors and symmetry groups.


The advent of relatively low cost computer graphics workstations has enabled us to teach undergraduates about various aspects of protein structure and function using molecular graphics to display and manipulate the structures.

There are many advantages to this approach:

i) Particular features of a structure can be examined in detail and accurate measurements made.

ii) Protein-protein and protein-ligand interactions can be dissected and docking processes simulated.

iii) Every student can have their "own molecule".

Some of our recent work devising practical to examine molecules such as haemoglobin, the D13 antibody-antigen complex, the photosynthetic reaction centre and the Met J repressor-operator complex using a variety of graphics packages and presentation software running on Silicon Graphics workstations will be described.