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 Preut, Fachbereich Chemie, Universität Dortmund, Postfach 50 05 00, D-4600 Dortmud 50, Germany.

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

1611 *Johannes Kepler*: De Nive Sexangula; **1661** *Niels Stensen*: Law of constancy of interfacial angles; **1891** *Evgraf Stepanovich Fedorov* and *Arthur Moritz Schoenflies*: 230 space groups; **1895** *Wilhelm Conrad Röntgen*: X-rays; **1912** *Walter Friedrich, Paul Knipping* and *Max von Laue*: X-ray diffraction; **1913** *William Henry Bragg* and *William Lawrence Bragg*: Crystal structure determination; **1934** *Arthur Lindo Patterson*: Heavy atom method; **1941** *Konrad Zuse*: Computer; **1947** : Synchrotron radiation; **1953** *Herbert Hauptman* and *Jerome Karle*: Direct methods; **1969** : First protein structure (Insulin).

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 *(Preut, H. (1989). Chemie in unserer Zeit,* **23** *, 121-129)* .

PS–19.01.10 TEACHING TENSORIAL PROPERTIES WITH REPRESENTATIONS. By V. Kopský, Department of Physics, University of the South Pacific, POBox 1168, Suva, Fiji.

Classical teaching of crystallography relies heavily on geometrical intuition. Though group theory accompanies crystallography from its early stages throughout the history of its development, the power and simplicity of group-theoretical methods, especially of representation theory, is not yet fully recognized.
This is to show how effective the approach of representation theory can be in calculation of tensorial properties. A standard approach is based on a direct inspection of invariance under the symmetry group. The procedure must be, in principle, performed separately for each tensor and each symmetry group though there exist some simplifying tricks, partly connected with parity arguments.
To show the full extent to which representation theory together with parity arguments can be exploited, let us consider four tensors: $\mathbf{u}$, $\varepsilon\mathbf{u}$, $\tau\mathbf{u}$, and $\varepsilon\tau\mathbf{u}$ under the action of magnetic point groups of the same oriented Laue class G (say $4_z2_x2_y$). Here $\mathbf{u}$ is a tensor which is invariant both under space inversion $\imath$ and magnetic (time) inversion $\imath'$ and hence also under combined inversion $\imath'' = \imath\imath'$.
ε is an i-pseudoscalar which changes its sign under space inversion $\imath$, τ is a c-scalar which changes its sign under time inversion $\imath'$ and $\varepsilon\tau$ is a c-pseudoscalar which changes its sign under both inversions.
G is the group of proper rotations which defines the Laue class.
It is clear that tensor $\mathbf{u}$ will have the same equilibrium form for all groups of the given Laue class. Four centrosymmetric groups ($4_z/m_zm_xm_{xy}$, $4_z/m_zm'_xm'_{xy}$, $4'_z/m_zm_xm'_{xy}$, and $4'_z/m_zm'_xm_{xy}$) contain explicitly $\imath$, four paramagnetic groups ($4_z2_x2_{xy}.1'$, $4_zm_xm_{xy}.1'$, $\overline{4}_z2_xm_{xy}.1'$, and $\overline{4}_zm_x2_{xy}.1'$) contain explicitly $\imath'$ and four groups ($4_z/m'_zm'_xm'_{xy}$, $4_z/m'_zm_xm_{xy}$, $4'_z/m'_zm_xm'_{xy}$, and $4'_z/m'_zm'_xm_{xy}$) contain explicitly $\imath''$. Finally, the centrosymmetric paramagnetic group $4_z/m_zm_xm_{xy}.1'$ contains explicitly all three inversions.
Parity arguments lead to selection rules. Tensor $\varepsilon\mathbf{u}$ is forbidden by groups which contain $\imath$ and/or $\imath''$, tensor $\tau\mathbf{u}$ by groups which contain $\imath'$ and/or $\imath''$, and tensor $\varepsilon\tau\mathbf{u}$ by groups which contain $\imath$ and/or $\imath'$. All tensors except $\mathbf{u}$ are therefore forbidden by the centrosymmetric paramagnetic group.

There are 16 magnetic point groups isomorphic with $4_z2_x2_{xy}$ which differ only in the way in which inversions are combined with proper rotation elements. The four scalars: 1, ε, τ, and $\varepsilon\tau$ transform by one-dimensional ireps Γ_1, Γ_2, Γ_3, and Γ_4, the first of which is identity, the remaining alternate. Since ε transforms by Γ_1 in groups $4_z2_x2_{xy}$, $4_z2'_x2'_{xy}$, $4'_z2'_x2_{xy}$, and $4'_z2_x2'_{xy}$, the tensor $\varepsilon\mathbf{u}$ will transform in the same way and hence it will have the same equilibrium form as the tensor $\mathbf{u}$ for these groups. The tensor $\tau\mathbf{u}$ will have this form in groups $4_z2_x2_{xy}$, $4_zm_xm_{xy}$, $\overline{4}_z2_xm_{xy}$, and $\overline{4}_zm_x2_{xy}$ and the tensor $\varepsilon\tau\mathbf{u}$ in groups $4_z2_x2_{xy}$, $4_zm'_xm'_{xy}$, $\overline{4}'_z2_xm'_{xy}$, and $\overline{4}'_zm'_x2_{xy}$.
The pseudoscalar ε transforms by Γ_2 in groups $4_zm_xm_{xy}$, $4_zm'_xm'_{xy}$, $4'_zm_xm'_{xy}$, and $4'_zm'_xm_{xy}$, c-scalar τ in groups $4_z2'_x2'_{xy}$, $4_zm'_xm'_{xy}$, $\overline{4}_z2'_xm'_{xy}$, and $\overline{4}_zm'_x2'_{xy}$, and c-pseudoscalar $\varepsilon\tau$ in groups $4_z2'_x2'_{xy}$, $4_zm_xm_{xy}$, $\overline{4}'_z2'_xm_{xy}$, and $\overline{4}'_zm_x2'_{xy}$. Accordingly, the corresponding tensors have the same transformation properties and hence equilibrium forms in respective groups. Analogously we use the ireps Γ_3 and Γ_4 and a slight modification applies to groups which contain some inversions explicitely.
This consideration has an interesting consequence. There exist only four possible nontrivial forms of tensors $\mathbf{u}$, $\varepsilon\mathbf{u}$, $\tau\mathbf{u}$, and $\varepsilon\tau\mathbf{u}$ in Laue class $4_z2_x2_{xy}$. Quite generally, the number of possible forms equals to the number of real one-dimensional ireps 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 $\mathbf{u}$. One table of transformation properties of tensors $\mathbf{u}$ under the group G together with a table of transformation properties of scalars under groups of Laue class G give then a transparent scheme which provides not only equilibrium tensors but also decomposition of tensors into bases of ireps. This relationship between tensors has been used recently (Grimmer, H. (1991). Acta Cryst. A**47**, 226-232), but the complete scheme has been described by the author a time ago (Kopský, V. (1979). Acta Cryst. A**35**, 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.

PS–19.01.11 TEACHING STUDENTS ABOUT PROTEIN STRUCTURE AND FUNCTION. D.A.Waller*, C.E.Sansom & A.J.Geddes, Department of Biochemistry and Molecular Biology, University of Leeds, Leeds, England

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 practicals to examine molecules such as haemoglobin, the D1.3 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.

PS–19.01.12 THE USE OF OPTICAL TRANSFORMS AS TEACHING AIDS. By T.R. Welberry*, Research School of Chemistry, Australian National University, GPO Box 4, Canberra City, ACT 0200, Australia.

