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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 Dortmund 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:  $u$ ,  $\epsilon u$ ,  $\tau u$ , and  $\epsilon \tau u$  under the action of magnetic point groups of the same oriented Laue class  $G$  (say  $4_2 2_x 2_y$ ). Here  $u$  is a tensor which is invariant both under space inversion  $i$  and magnetic (time) inversion  $e'$  and hence also under combined inversion  $i' = ie'$ .  $\epsilon$  is an  $i$ -pseudoscalar which changes its sign under space inversion  $i$ ,  $\tau$  is a  $c$ -scalar which changes its sign under time inversion  $e'$  and  $\epsilon \tau$  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  $u$  will have the same equilibrium form for all groups of the given Laue class. Four centrosymmetric groups ( $4_2/m_2 m_x m_{xy}$ ,  $4_2/m_2 m'_x m'_{xy}$ ,  $4'_2/m_2 m_x m_{xy}$ , and  $4'_2/m_2 m'_x m'_{xy}$ ) contain explicitly  $i$ , four paramagnetic groups ( $4_2 2_x 2_y.1'$ ,  $4_2 m_x m_{xy}.1'$ ,  $4_2 2_x m_{xy}.1'$ , and  $4_2 m_x 2_{xy}.1'$ ) contain explicitly  $e'$  and four groups ( $4_2/m'_2 m'_x m'_{xy}$ ,  $4_2/m'_2 m_x m_{xy}$ ,  $4'_2/m'_2 m_x m_{xy}$ , and  $4'_2/m'_2 m'_x m'_{xy}$ ) contain explicitly  $i'$ . Finally, the centrosymmetric paramagnetic group  $4_2/m_2 m_x m_{xy}.1'$  contains explicitly all three inversions.

Parity arguments lead to selection rules. Tensor  $\epsilon u$  is forbidden by groups which contain  $i$  and/or  $i'$ , tensor  $\tau u$  by groups which contain  $e'$  and/or  $i'$ , and tensor  $\epsilon \tau u$  by groups which contain  $i$  and/or  $e'$ . All tensors except  $u$  are therefore forbidden by the centrosymmetric paramagnetic group.

There are 16 magnetic point groups isomorphic with  $4_2 2_x 2_y$  which differ only in the way in which inversions are combined with proper rotation elements. The four scalars:  $1$ ,  $\epsilon$ ,  $\tau$ , and  $\epsilon \tau$  transform by one-dimensional irreps  $\Gamma_1$ ,  $\Gamma_2$ ,  $\Gamma_3$ , and  $\Gamma_4$ , the first of which is identity, the remaining alternate. Since  $\epsilon$  transforms by  $\Gamma_1$  in groups  $4_2 2_x 2_y$ ,  $4_2 2'_x 2'_{xy}$ ,  $4'_2 2'_x 2'_{xy}$ , and  $4'_2 2_x 2'_{xy}$ , the tensor  $\epsilon u$  will transform in the same way and hence it will have the same equilibrium form as the tensor  $u$  for these groups. The tensor  $\tau u$  will have this form in groups  $4_2 2_x 2_y$ ,  $4_2 m_x m_{xy}$ ,  $4_2 2_x m_{xy}$ , and  $4_2 m_x 2_{xy}$  and the tensor  $\epsilon \tau u$  in groups  $4_2 2_x 2_y$ ,  $4_2 m'_x m'_{xy}$ ,  $4'_2 2_x m'_{xy}$ , and  $4'_2 m'_x 2_{xy}$ .

The pseudoscalar  $\epsilon$  transforms by  $\Gamma_2$  in groups  $4_2 m_x m_{xy}$ ,  $4_2 m'_x m'_{xy}$ ,  $4'_2 m_x m'_{xy}$ , and  $4'_2 m'_x m_{xy}$ ,  $c$ -scalar  $\tau$  in groups  $4_2 2'_x 2'_{xy}$ ,  $4_2 m'_x m'_{xy}$ ,  $4_2 2'_x m'_{xy}$ , and  $4_2 m'_x 2'_{xy}$ , and  $c$ -pseudoscalar  $\epsilon \tau$  in groups  $4_2 2'_x 2'_{xy}$ ,  $4_2 m_x m_{xy}$ ,  $4_2 2'_x m_{xy}$ , and  $4_2 m_x 2'_{xy}$ . Accordingly, the corresponding tensors have the same transformation properties and hence equilibrium forms in respective groups. Analogously we use the irreps  $\Gamma_3$  and  $\Gamma_4$  and a slight modification applies to groups which contain some inversions explicitly.

This consideration has an interesting consequence. There exist only four possible nontrivial forms of tensors  $u$ ,  $\epsilon u$ ,  $\tau u$ , and  $\epsilon \tau u$  in Laue class  $4_2 2_x 2_y$ . 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  $u$ . One table of transformation properties of tensors  $u$  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 irreps. This relationship between tensors has been used recently (Grimmer, H. (1991). *Acta Cryst.* A47, 226-232), but the complete scheme has been described by the author a time ago (Kopský, 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.

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.

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The idea of using optical analogues (or Optical Transforms) to aid in the interpretation of X-ray diffraction patterns originated with Sir Lawrence Bragg round about 1938, and the method has developed considerably since that time. Prior to the advent of digital computers calculation of the diffraction pattern of even a fairly simple crystal structure was an enormous task, and use of optical diffraction from a model had obvious benefits, particularly for testing trial structures. With the advent of computers the task of obtaining a calculated diffraction pattern of an ordered crystal structure for comparison with observed measurements became a rather trivial exercise and use of the optical method for this purpose began to fall into disuse. On the other hand for the structural elucidation of disordered structures, amorphous materials and even liquids the transform method has continued to be used even though the diffraction pattern of even the most complex structural model can in principle be calculated quite readily with modern computers.

Optical Transforms are particularly useful in a teaching context where the student is able to verify for him/herself the relationship between a real-space object and its diffraction pattern. In this demonstration we present examples of optical diffraction masks, the structural details of which can be inspected with the use of an ordinary micro-fiche viewer or 35mm slide projector, and whose diffraction patterns can be observed using only simple apparatus. A varied selection of masks will be available to demonstrate the diversity of diffraction effects which may be achieved by the technique.

In recent years we have sought to develop methods to allow the routine production of optical diffraction masks (or screens) for use as aids in the interpretation of X-ray or electron diffraction patterns. We are now able to produce, rapidly and easily, an optical diffraction mask which is a good representation of almost any real diffraction problem encountered with X-rays or electrons. Among the diverse range of problems that we have studied with the aid of such diffraction masks are: short-range order in molecular crystals; size-effect distortions in alloys; thermal and disorder diffuse scattering in minerals; small-angle scattering in microemulsions; fluctuations of local order in liquids; quasi-crystals.

**PS-19.01.13 CENET, A CRYSTALLOGRAPHIC NETWORK IN THE EUROPEAN COMMUNITY ERASMUS PROGRAM.** By Henk Schenk\*, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam

The Erasmus scheme of the European Community provides opportunities for tertiary education to exchange students and staff and to set up new teaching. Emphasis lies on the student exchanges. Students are studying in between 3 and 12 months in another country within the European Community. The most important constraint for these stays is that the full period should be recognized by the home-university for the curriculum of the student. Since a few years the Erasmus scheme is also open to the Efta countries. At present crystallography groups of 10 universities work together in the CENET Erasmus project: Amsterdam, Bologna (Lodovico Riva di Sanseverino), Bordeaux (Michel Hospital), Copenhagen (Ingrid K. Larsen), Dublin (Christine Cardin), Edinburgh (Bob Gould), Erlangen (Hans Burzlaff), Leuven (Camiel de Ranter), Lisbon (Maria Armenia Carrondo) and Thessaloniki (Panos Rentzeperis), originating from the faculties of chemistry, physics, pharmacy and geology. In CENET students of the 4th, 5th and 6th year at University are being

exchanged for 3 months. This has the advantage that their stay abroad can easily be recognized as part of the research period they have to complete in nearly all curricula of the participating universities. Three students are being exchanged per group, they go to different countries and the visiting students not necessarily originate from the same countries, it rather depends on the individual research interests. To achieve this there is a complicated exchange scheme, supervised by the Amsterdam group, run via Email. The results of the student exchanges are very encouraging. The main result is an increase of mobility; it had been always possible for active students to follow courses in other countries, but mostly they lost time by doing so. In this scheme where it is obligatory for the universities involved to recognize foreign periods in the own curricula, this problem has been overcome. As a result all students may include a foreign period in their curriculum without any penalty. Individual students appreciate the possibilities very much. The teaching staff sees as major advantages the increased self-reliance of individual students and the international orientation of their groups.

**PS-19.01.14 SYMBAD, A CAI PROGRAM FOR TEACHING THE SYMBOLIC ADDITION METHOD.** By Yuan-Fang Wang\* and Henk Schenk, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

Since Direct Methods are still of growing importance as a tool of solving crystal structures from single crystal data and most program systems for Direct Methods are not very transparent, we developed a small Computer Assisted Instruction (CAI) for the TRS80, in which the chemistry students are guided to work with the Symbolic Addition method. The main task of the computer is to teach the student direct methods and to do the administration, while the students learn to take the essential decisions and is doing a phase extension process. With these experiences as background we wrote a CAI system in BASIC for PC's which allows more flexibility to the user. The program system is menu driven with an integrated manual. Input data for a projection of a structure are provided on disk, however, it is easy to create a local file of a suitable structure in which the overlap in projection is minimal as Direct Methods function better at atomic resolution. The program can handle projections with triclinic centrosymmetric symmetry only, and as a result in particular structures with one short axis can be used successfully.

The menu gives the following options:

- Manual: A short explanation of the method and how to handle it.
  - Input data: The student can choose between an input by keyboard or by disk. Keyboard data can be saved on disk for future use.
  - Generation of triplets: is fully automatic and generates triplets with an E3 value higher than a limit value, to be given by the student.
  - Symbolic addition: In this part the computer does only the administration; the student makes the decisions, i.e. she/he chooses the sign/symbol of the reflections in the starting set and decides whether the calculated phase of a reflection is being accepted.
  - E-map: The student defines the values of the symbols and then the program calculates on the basis of the phases E-maps.
- The program is accompanied by a programmed text, which teaches the triplet relation along the lines of chapter 1 of the proceedings of this conference and uses a similar approach to teach the principles of the symbolic addition method. The work has been sponsored in part by the Erasmus Scheme of the European Community.

**PS-19.01.15 AFRICAN PATCHWORK PATTERNS AS SYMMETRY TEACHING TOOLS.** By Yves BILLIET\* and Marie-Paule BILLIET-NYBELEN, Departement de Chimie, Faculté des Sciences, Boite Postale 825, Niamey, Niger.