

Society of Crystallographers

in

Australia

Newsletter No. 6

1983

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OFFICE BEARERS

President: B.M.K. Gatehouse (Monash Univ.)
Vice President: T.M. Sabine (NSWIT)
Secretary: R.J. Hill (CSIRO Min. Chem.)
Treasurer: M.F. Mackay (LaTrobe Univ.)
Council: Z. Barnea (Melb. Univ.)
W.T. Robinson (Univ. Canterbury, N.Z.)
F.H. Moore (AINSE)
E.N. Maslen (Univ. WA) (immediate past President)

Standing Committees (*Chairperson)

Electron Diffraction: P. Goodman (CSIRO Chem. Phys.)*
A.W.S. Johnson (CSIRO Chem. Phys.)
J.R.J. Sellar (ANU)

X-ray Diffraction: I.E. Grey (CSIRO Min. Chem.)*
J.M. Guss (Univ. Sydney)
S.W. Wilkins (CSIRO Chem. Phys.)

Neutron Diffraction: V.J. James (Univ. NSW)*
C.J. Howard (AAEC)
T.J. Hicks (Monash Univ.)

Computing: S.R. Hall (Univ. WA)*
N.W. Isaacs (St Vincents Sch. Med. Res.)
A.D. Rae (Univ. NSW)

Nominations: E.W. Radoslovich (CSIRO Soils)*
S.L. Mair (CSIRO Chem. Phys.)
M.R. Snow (Univ. Adelaide)

Newsletter Editor: R.J. Hill
CSIRO Div. Mineral Chemistry
PO Box 124, Port Melbourne
Victoria, 3207

ELECTION OF OFFICERS AND STANDING COMMITTEES

In accordance with Rule IV, Section 1 of the SCA Constitution, the Nominations Committee has proposed the following list of nominations for all the positions for which vacancies will occur after the Business Meeting at Morpeth in August. The Secretary now invites additional nominations for these positions to be submitted over the signatures of two SCA members not later than April 30, 1983.

<u>Position</u>	<u>Nomination</u>
Vice President	Dr S.R. Hall (Univ. WA)
Secretary	Dr R.J. Hill (CSIRO, Min. Chem.)
Treasurer	Dr M.F. Mackay (LaTrobe Univ.)
Council	Dr R.W. Cheary (NSWIT)
Electron diffraction	Dr R.A. Eggleton (ANU)
X-ray diffraction	Dr J.N. Varghese (Univ. WA) ←
Neutron diffraction	Dr C.H.L. Kennard (Univ. Q)
Computing	Dr G.M. McLaughlin (ANU)
Nominations	Dr J. Epstein (ANU)

SCA COUNCIL MEETING, JANUARY 1983

Council of the SCA met in January 1983 to consider several matters of relevance to the crystallographic community in Australia. A brief summary of some of the results of this Council meeting follows:

- (i) Incorporation of the SCA has required amendments to be made to the Constitution. Council's recommended changes will be presented to the membership for approval and comments etc at Morpeth.
- (ii) The SCA has now officially supported the formation of a new I.U.Cr. Commission on Structural Analysis of Organic and Biologically Active Small Molecules.
- (iii) Dr S.R. Hall has been nominated to act as spokesman for the SCA at the Kyoto Computing School in August, 1983, in support of the formation of a South-East Asian Regional Group of the I.U.Cr.
- (iv) The Society's financial statements will in future be audited. This measure was considered desirable in view of the anticipated increase in revenue arising from the lead-up to the 1987 I.U.Cr. Congress.
- (v) Student participation at the forthcoming Crystal 14 meeting is to be encouraged by making available a limited amount of financial support for SCA student members attending the meeting, and by the awarding of a book prize to the student with the best oral or poster contribution.

PERSONALIA

Dr E.R. Segnit of the CSIRO Division of Mineral Chemistry has been elected to the 10 person Council of the International Mineralogical Association. The IMA is the reference point for worldwide mineralogical data and research and it is the first occasion on which an Australian has been so honoured.

Dr Mogens Lehmann from the ILL, Grenoble, will be a joint visitor at the CSIRO Division of Chemical Physics, Clayton, and the Dept. of Physics, Monash University, for all of April, 1983. He will be giving an AIP lecture at 8 pm on April 21 at the Hercus Theatre, Dept. of Physics, Melbourne University, entitled "New Directions for

Neutron Scattering at the ILL". He will spend the first week of May visiting the AAEC Research Establishment at Lucas Heights, NSW.

A warm welcome is extended to Dr P.R. Prager of the Dept. of Physics at Melbourne University, who has recently become a member of the SCA.

WADSLEYITE

Members of the SCA (and others) will be particularly pleased to hear that Dr A.D. (Dave) Wadsley, one of Australia's most outstanding crystal chemists/crystallographers has been honoured, some 15 years after his death, by the naming of a mineral after him. The new mineral, Wadsleyite, is an intermediate phase in the transformation of olivine to spinel and has the composition $(\text{Mg}_{1.5}\text{Fe}_{0.5})\text{SiO}_4$. It was discovered in the Peace River (Alberta) Meteorite.

Other minerals named after Australian crystallographers/mineralogists include:

Aldermanite	$\text{Mg}_5\text{Al}_{12}(\text{PO}_4)_8(\text{OH})_{22} \cdot n\text{H}_2\text{O}$
Baylissite	$\text{K}_2\text{Mg}(\text{CO}_3)_2 \cdot 4\text{H}_2\text{O}$
Davidite	$(\text{Fe}, \text{La}, \text{U}, \text{Ca})_6(\text{Ti}, \text{Fe})_{15}(\text{O}, \text{OH})_{36}$
Bowleyite	$3(\text{Ca}, \text{Be})\text{O} \cdot 2\text{Al}_2\text{O}_3 \cdot 3\text{SiO}_2 \cdot 2\text{H}_2\text{O}$
Braggite	$(\text{Pt}, \text{Pd}, \text{Ni})\text{S}$
Formanite	YTao_4
Georgeite	$\text{Cu}_5(\text{CO}_3)_3(\text{OH})_4 \cdot 6\text{H}_2\text{O}$
Jeppelite	$(\text{K}, \text{Ba})_2(\text{Ti}, \text{Fe})_6\text{O}_{13}$
Kingite	$\text{Al}_3(\text{PO}_4)_2(\text{OH}, \text{F})_3 \cdot 9\text{H}_2\text{O}$
Kleemanite	$\text{ZnAl}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 3\text{H}_2\text{O}$
Loveringite	$(\text{Ca}, \text{Ce})(\text{Ti}, \text{Fe}, \text{Cr}, \text{Mg})_{21}\text{O}_{38}$
Majorite	$\text{Mg}_3(\text{Fe}, \text{Al}, \text{Si})_2(\text{SiO}_4)_3$
Mawsonite	$\text{Cu}_6\text{Fe}_2\text{SnS}_8$
Priderite	$(\text{K}, \text{Ba})(\text{Ti}, \text{Fe})_8\text{O}_{16}$
Raspite	PbWO_4
Ringwoodite	$(\text{Mg}, \text{Fe})_2\text{SiO}_4$
Simpsonite	$\text{Al}_4(\text{Ta}, \text{Nb})_3(\text{O}, \text{OH}, \text{F})_{14}$
Skinnerite	Cu_3SbS_3
Stillwellite	$(\text{Ce}, \text{La}, \text{Ca})\text{BSiO}_5$
Threadgoldite	$\text{Al}(\text{UO}_2)_2(\text{PO}_4)_2(\text{OH}) \cdot 8\text{H}_2\text{O}$

Incidentally, with politics on everyone's mind at the moment the mineral Holtite (with a formula too complex to mention here) was named after the Rt. Hon. Harold Edward Holt (1908-1967), Prime Minister of Australia 1966-7. Readers should note that the surnames Whitlam, Fraser and Hawke are as yet unused in the mineralogical world!

Structure of life

Aaron Klug of the Medical Research Council Laboratory of Molecular Biology in Cambridge has won this year's Nobel Prize for Chemistry.

Klug first arrived in Cambridge as a graduate student from South Africa in 1949; 15 years later he went to Birkbeck College in London and he returned to Cambridge in 1962. At Birkbeck, Klug developed an interest in the structure of viruses and some of his first studies were on tobacco mosaic virus (TMV). At first he employed X-ray diffraction, collaborating with Rosalind Franklin — whose contribution to the solution of the structure of DNA he has always championed.

To supplement X-ray studies, Klug employed high resolution electron microscopy to produce models of the structure of helical and spherical viruses. A key concept to emerge from that work was

the "principle of quasi-equivalence" of subunit packing of the protein particles of viruses. Don Caspar (now at Brandeis University in Massachusetts) and Klug put forward that principle in 1962.

After his return to Cambridge in 1962, Klug continued to devote much of his attention to TMV to understand further the interactions between protein and nucleic acids. Three classic papers on the assembly of the RNA and protein components of TMV into the functioning virus were published in *Nature New Biology* in 1971. And ever higher resolution structures of the TMV disc protein have continued to appear, the ultimate being the 2.8 Angstrom structure of 1978 (*Nature* 276, 362).

The Nobel prize citation for Klug's prize rightly is not confined to his contributions towards understanding the structure of complexes of proteins and nucleic acids, notably TMV but more recently also the

nucleosome, the repeating structural unit of chromatin. Instead the citation is also for his development of crystallographic electron microscopy. That technique arose from Klug's realization that the diffraction methods of X-ray crystallography could be applied to electron microscopic images of regular biological structures. The technique emerged in the mid-1960s, at first using optical diffraction, but by 1968 Klug and David de Rosier were reconstructing three dimensional images by computer analysis of Fourier transforms of negatively stained electron microscopic images. Among structures to have yielded to Klug and these techniques have been tail fibre of bacteriophage T4, thin filaments of muscles and the nucleosome.

Others may have contributed as much as Klug to individual accomplishments but the Nobel committee has recognized that the whole is greater than the sum of the parts.

Peter Newmark

(from *Nature* 299, 672, 1982)

Klug has transformed the interpretation of electron micrographs from a subjective art into an exact science and has used that science to unravel the structures of viruses and chromosomes. He applied to electron microscopy principles of physical optics similar to those used in X-ray crystallography.

Klug's methods require that the specimen possesses some form of periodicity such as is often present, or can be induced, in biological structures. If an electron micrograph of such a specimen is subjected to Fourier analysis, the Fourier terms due to the regularly repeating features stand out from the general noise that is due to the irregular distortions of individual molecules. Both the amplitudes and phases of the Fourier terms can be measured. The effects on the image of spherical aberration and underfocussing can be measured independently, and the results of these measurements can be used to apply corrections to the Fourier terms. Finally, the corrected Fourier terms can be recombined to form an image of the specimen. At first Klug and his collaborators used optical methods for image analysis and recombination, but later they found densitometry and digitizing of the image, followed by Fourier analysis by computer, to be more powerful and to facilitate correction for electron optical artefacts.

Two-dimensional electron micrographs tend to be confused by the overlapping of the many features that lie within the depth of focus of the objective lens; for many years this was regarded as a limitation inherent in electron microscopy. In the X-ray analysis of crystals three-dimensional images are built up by combining the Fourier terms of images projected in many different directions. D. De Rosier and Klug argued that similar methods must be applicable to electron microscopy. If a series of images of the same specimen is taken at different angles of tilt and each image is transformed into its Fourier terms, then recombination of all these terms builds up a three-dimensional image.

Before any of this work had started D. Caspar and Klug predicted that the protein shells of spherical viruses, such as polio virus, can be classified according to their symmetry, rather like the planar point groups. Klug's advances in electron microscopy allowed him and his collaborators, principally J. T. Finch and R. A. Crowther, to test and confirm that theory, and to obtain well-resolved three-dimensional images of many other large biological molecules. Their most recent and spectacular discovery concerns the regular beaded structure of chromosomes, each bead consisting of a protein spool around which are wound two turns of double-helical DNA.

M. F. Perutz

(from *ACA Newsletter*, 14, 2, 1983)

THE BERTRAM E. WARREN AWARD

The Bertram E. Warren Award in diffraction physics was presented to Benjamin Post of the Polytechnic Institute of New York. The Award, given every three years by the American Crystallographic Association, recognizes an important contribution to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques and consists of a certificate and a \$1000 cash prize.

Post was cited for "his contributions to simultaneous many-beam dynamical diffraction theory and the application

of these results to a solution of the phase problem of x-ray crystallography."

After obtaining his PhD in physical chemistry from the Polytechnic Institute of New York in 1949, Post continued his research there and is now professor of physics and chemistry. He served as president of the American Crystallographic Association from 1966 to 1967.

His research interests have encompassed many areas of crystallography, including his early work in low-temperature diffraction, crystal structure determination and polymorphism, and later research in dynamical diffraction and *n*-beam simultaneous diffraction. One of Post's most important recent contributions involved the "phase problem." Determining crystal structure by x-ray methods requires knowledge of both the relative phases and the amplitudes of beams diffracted from the crystal, but only the amplitudes are directly measurable; it was generally believed that information about the phases was experimentally inaccessible. Post showed that when two or more sets of planes diffract simultaneously, the distribution of diffracted intensities depends on the phases of the reflections involved. Phases can thus be determined experimentally.

POST



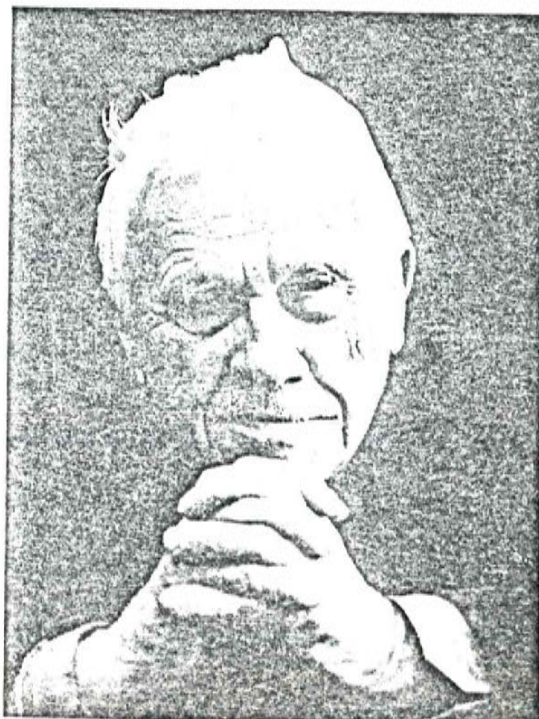
(from *Physics Today*, Nov. 1982, p 83)

OBITUARY OF N.V. BELOV

Nikolay Vasilyevich Belov

14 December 1891–6 March 1982

The international community of crystallographers suffered a heavy loss on 6 March 1982 when Professor Nikolay Vasilyevich Belov, a full member of the USSR Academy of Sciences and one of the world's greatest crystallographers, died suddenly. N. V. Belov had been full of energy, taking his usual active part in the work of the academic Institute of Crystallography and Moscow State University, until the previous day. The photograph above portrays him two days before his death.



N. V. Belov was born on 14 December 1891 in Yanov (now in Poland) into a physician's family. The family moved to Ovruch (North Ukraine) in 1900, and when Belov talked about his childhood it was to reminisce about this small town. Belov finished Gymnasium in Warsaw and entered St. Petersburg Polytechnic Institute in 1910.

His studies were interrupted by the First World War and then by the Revolution and the Civil War in Russia. He returned to Ovruch and took an active part in reconstructing a city economy devastated by war. It was not until 1921 that he was able to complete his education. He returned to Leningrad in 1924 and joined Lenkozhrest (Leningrad Raw Leather Trust); he later headed its Central Chemical Laboratory and also the Chemical Laboratory of the Institute on the Study of the North. His zest for science in this period was manifested by the publication of over 70 popular scientific articles in *Priroda* (Nature) from 1928 to 1932. A. E. Fersman, the Editor-in-Chief of this journal, invited N. V. Belov to join the Lomonosov Institute of the USSR Academy of Sciences.

Practical use of the great Kola Peninsula deposits was, at that time, an important matter. Belov proceeded to investigate the main Khibiny minerals, nepheline and apatite. He soon published a number of papers on nepheline technology in the tanning, textile, paper and woodworking industries and also proposed an original method for extracting rare earths from apatites.

The Academy of Sciences moved to Moscow in 1934 and Belov followed in 1936. Shortly thereafter he transferred from the Geochemical Department of the Lomonosov Institute to its Crystallographic Department headed by Professor A. V. Shubnikov. It was during this period that Belov's scientific interests concentrated on crystal chemistry, structural mineralogy and the X-ray analysis of crystals. He set himself the goal of creating a unique crystallochemical understanding of the atomic structure of inorganic compounds. He elaborated the theory of closest-packed anionic spheres and analyzed possible schemes for the population of the resulting octahedral and tetrahedral interstices by cations. The results of these investigations led to his doctoral dissertation, which he defended in 1943, and later to his monograph *Structure of Ionic Crystals and Metallic Phases* published in 1947. The first structural solutions of rather complicated silicates were carried out by Belov and his students by the trial-and-error method using the principle of closest packing.

More complicated objects of investigation and new ideas in the field of Patterson and direct methods of determining crystal structures pushed trial-and-error methods into the background. Belov became an enthusiast for new methods and one (together with his students) of their active creators.

The silicates played a major part in his investigations. If W. L. Bragg was the founder of the crystal chemistry of silicates, N. V. Belov was the creator of its 'Second Chapter', in which silicates with such large cations as calcium, potassium, sodium, and rare-earth elements are of major importance. He later became interested in borates, germanates, sulphides, sulphates and other representatives of the mineral kingdom. He and his students determined the structures of more than 500 naturally occurring and synthetic compounds. On the basis of structural representation, he analyzed the geochemical processes in the earth's crust and the problem of isomorphism.

Belov's works in the field of symmetry are well known. He presented the simplest 'visual' derivation of the 230 space groups (suitable for student audiences) and, together with his students, derived the 1651 Shubnikov black-and-white symmetry groups. With his students, he was the author of fundamental works on colour symmetry and investigations in the field of four-dimensional space-group symmetry.

N. V. Belov was elected a Corresponding Member in 1946 and a Full Member in 1953 of the USSR Academy of Sciences.

Nikolay Vasilyevich devoted much time and effort to pedagogical activities. He was professor in both Gorky and Moscow Universities; he had been head of the Chair of Crystallography and Crystal Chemistry of the Geological Department of Moscow University since 1961. He was the founder of the Soviet structural school. Under his guidance, more than 150 specialists prepared and defended their doctoral and candidate dissertations. The graduates of Belov's school are now scientifically active in Moscow, Gorky, Novosibirsk, Baku, Kishinev, Ashkhabad and many other cities of the Soviet Union.

N. V. Belov was Editor-in-Chief of *Kristallografiya* until his last days; he had been permanent Chairman of the USSR National Committee of Crystallography since 1955. He was a member of the Executive Committee of the International Union of Crystallography from 1954 to 1963 and from 1966 to 1972; he was Vice-President from 1960 to 1963 and President of the Union from 1966 to 1969. He was an Honorary Member of the Mineralogical Societies of the USSR, USA, Great Britain and France; of the Geological Society of the DDR, and was a Foreign Member of the Polish Academy of Sciences. Wrocław University conferred on him the honorary degree of Doctor of Science.

N. V. Belov was honoured with the title of Hero of Socialist Labour and was awarded four Orders of Lenin, the order of the October Revolution and the Red Banner of Labour, as well as many medals for his scientific and pedagogical achievements. His enormous contributions to science were recognized by Lenin and State Prizes. He was also awarded the Lomonosov Gold Medal – the highest honour within the patronage of the Academy of Sciences of the USSR.

His fine human qualities were most admirable. It was typical that, until the day before he died, he was available to any who needed his advice and support in science as well as in everyday life.

His knowledge, not only of science but also of literature, art and history, was indeed encyclopedic. His scientific publications have a charm of style that cannot be found in other authors' work.

Nikolay Vasilyevich Belov – the great expert in science who headed Soviet Crystallography, the educator of several generations of crystallographers, the scientist of enormous erudition, active and vigorous until his last day, a person of rare charm, modesty and kindness – will remain for ever in the history of science and will always be prominent in the memory of those who were fortunate enough to know him.

B. K. VAINSHTEIN
V. I. SIMONOV

Acta Cryst. (1982). A38, 561–562

FORTHCOMING MEETINGS

Meetings of general interest to SCA members coming up in the near future include:

- May 16–20, 1983: 5th National School and Conference on X-ray Analysis, Melbourne. Contact: Mr R.A. Coyle, PO Box 90, Parkville 3052, Victoria (see below).
- June 12–16, 1983: Euehem Conference on HREM in Solid State Chemistry, Skepparholmen near Stockholm, Sweden. Contact: Dr Per Stenson, Swedish Nat. Committee for Chemistry, Upplandsgatan 6A, S-111 23 Stockholm, Sweden.
- July 4–8, 1983: 4th International Conference on Solid State Ionics, Grenoble, France. Contact: M. Kleitz, SSI 83, ENSEEG, BP 44, 38 401 Saint Martin d'Heres, France.
- July 11–15, 1983: Gordon Conference on Electron Distribution and Chemical Bonding, Plymouth State College, New Hampshire. Contact: Prof. G.A. Jeffrey, Dept of Crystallography, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA.
- July 20–30, 1983: School on Direct Methods and Macromolecular Crystallography, Buffalo, New York. Contact: Dr Jane F. Griffin, Medical Foundation of Buffalo, 73 High Street, Buffalo, New York 14203, USA.
- August 1–5, 1983: ACA Meeting, Snowmass, Colorado. Contact: Prof. R.D. Witters, Dept of Chemistry, Colorado School of Mines, Golden, Colorado 80401, USA.
- August 8–12, 1983: 8th European Crystallographic Meeting, Liege, Belgium. Contact: Leon Dupont, Institute de Physique B5, Universite de Liege Sart-Tilman, B-4000, Liege, Belgium.
- August 18–27, 1983: International Summer School on Crystallographic Computing, Kyoto, Japan. Contact: Dr S.R. Hall, Crystallography Centre, University of WA, Nedlands 6009.

- Sept. 5-10, 1983: Eighth Iberoamericano Congress of Crystallography, Buenos Aires and La Plata, Argentina. Contact: Dr Maria A.R. de Benyacar, Avda. del Libertador 8250, 1429 Buenos Aires, Argentina.
- Sept. 12-14, 1983: Third National Conference on Synchrotron Radiation Instrumentation, Brookhaven National Laboratory. Contact: Dr William Thomlinson, Chairman, Brookhaven Nat. Lab., Nat. Synchrotron Light Source, Upton, Long Island, New York 11973, USA.
- Nov. 24 & 25, 1983: RACI Solid State Division Two-day Symposium, Univ. of Melbourne. Contact: Mr H. Jaeger, CSIRO Division of Materials Science, Univ. of Melbourne, Parkville 3052.
- Jan. 22-26, 1984: 12th Conference of the RACI COMO Division, University of Tasmania, Hobart. Contact: Dr P.W. Smith, Chemistry Dept., Univ. of Tasmania, Box 252C, GPO, Hobart 7001.
- May 6-20, 1984: International School on Direct Methods of Solving Crystal Structures, Erice, Italy. Contact: Prof. L. Riva di Sanseverino, Istituto di Mineralogia, Piazza di Porta San Donato I, 40127 Bologna, Italy.
- August 9-18, 1984: I.U.Cr. 13th Congress, Hamburg, Germany. Contact: Dr H. Saalfeld, Mineralogisch-Petrogr. Inst., Universitat, Grindelallee 48, D-2000 Hamburg (see below).

CRYSTAL 14

Remember that the next SCA meeting (Crystal 14) is being held at the Morpeth Conference Centre, near Maitland in the Hunter Valley from Aug. 30 to Sept. 2, 1983. Even if the meeting was not being held at that time it would still be a great place to spend a few days R and R. So, if you have not sent off your Intention to Attend form, dig up the last Newsletter or just send Rick Tietze a note at the Dept. of Chemistry, University of Newcastle, before you forget.

Supervisors please note that there will be some limited financial assistance for (SCA) students attending Crystal 14, and a book prize will be awarded to the best student paper presented at the meeting.

The tentative program of invited speakers, and the titles of their talks are as follows (timetable only preliminary):

Tues., Aug. 30, pm:	Registration and Mixer	
Wed., Aug. 31, am:	Dr U.W. Arndt	"Area detectors"
	Dr S.W. Wilkins	"An information-theoretical approach to the crystallographic inversion problem"
pm:	Dr A.H. White	"Structural relationships in coinage metal halide/base complexes"
	Prof. B.G. Hyde	"An alternative, novel view of some ionic/mineral crystal structures"

Thurs., Sept. 1, am:	Dr S.R. Hall	"On structure determination problems"
	Dr E.N. Maslen	"Charge density studies of rare earth compounds"
pm:	Dr M.R. Snow	"Managing crystallographic data on a minicomputer"
	Dinner at Rothbury Estate	
Fri., Sept. 2, am:	Dr I.E. Grey	"Structure analysis by non classical methods"
	Dr P.M. Colman	"Structure of Neuraminidase"

AXAA 83

The Fifth Australasian Schools and Conference on X-ray Analysis with sessions on Surface Analysis will be held at the Victorian College of Pharmacy, 381 Royal Parade, Parkville, from 16th-20th May 1981.

Schools on X-ray Diffraction, X-ray Fluorescence and Surface Analysis will be held concurrently from 9.00 am Monday, 16th May to 12.30 pm Wednesday 18th May, followed by visits to Industrial/Research Organizations and a concurrent Workshop on Computer Search and Match techniques. The Conference sessions will be run from 9.00 Thursday, 19th May to 3.00 pm Friday, 20th May with invited Plenary papers by K. Norrish (CSIRO Div. of Soils, Adelaide), C.D. Hubbard (National Bureau of Standards, Washington), B.F. Phillips (Perkin-Elmer Physical Electronics Div., Maine), M.A. Short (Occidental Res. Corp., California) and F.P. Robotham (Health Commission of Victoria).

For further details of the program and registration contact:

The Conference Secretary
AXAA 83
PO Box 90
Parkville. Vic. 3052.

or phone Pat Wright: (03) 560 7066

13th CONGRESS OF THE I.U.Cr.

Dr H.C. Freeman has been invited to be a member of the Programme Committee for the 13th Congress of the I.U.Cr. which is to be held in Hamburg in August 1984. As such he would be pleased to hear from any member of the SCA who has strong views on the format of the Congress or suggestions concerning the programme. The Programme Committee is to meet in August of this year, so your comments or suggestions would be welcome as soon as possible. Dr Freeman can be contacted through the Secretary of the SCA or directly at the Dept. of Inorganic Chemistry, Univ. of Sydney, NSW 2006: 02-692 2757.

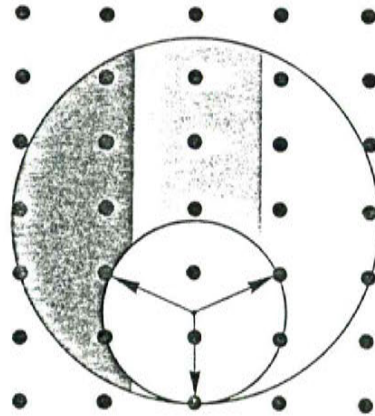
Please give this matter your serious consideration since we will have to be doing the same thing, at much closer quarters, for the 14th Congress in 1987 in Perth.

A copy of the First Announcement of the 13th Congress is reproduced below:

FIRST ANNOUNCEMENT JANUARY 1983

XIIITH CONGRESS AND GENERAL ASSEMBLY

INTERNATIONAL UNION OF CRYSTALLOGRAPHY



9-18 AUGUST 1984
CONGRESS CENTRUM HAMBURG
Hamburg, Federal Republic of Germany

Sponsored by the
Deutsche Forschungsgemeinschaft
(DFG)
and
Freie und Hansestadt Hamburg

You are cordially invited by the
Arbeitsgemeinschaft Kristallographie
(AGK) of the
Federal Republic of Germany
to attend the

XIIIth Congress and General Assembly of
the International Union of Crystallography
to be held in Hamburg at the Congress Cen-
trum Hamburg (CCH). Registration will begin
on Wednesday, 8 August 1984. The sessions
will continue until 18 August.

PROGRAMME

The scientific programme will include invited
general lectures, invited oral papers and open
Commission meetings. Most contributed
papers will be presented in poster sessions.
Commercial and non-commercial apparatus
will be exhibited and crystallographic data file
demonstrations are planned.

SUBJECTS

The congress will cover recent advances in all
aspects of crystallography. It is anticipated
that the following areas will be represented:

GENERAL TOPICS

Anomalous scattering
Atomic scale mechanisms of physical, chemi-
cal or biological properties
Applied crystallography
Computing statistics
Crystal chemistry
Crystal physics
Crystal growth and morphology
Diffraction theory
Dynamical diffraction
Education and data retrieval
Electron density studies
Electron diffraction and microscopy
EXAFS and near-edge spectroscopy
Instrumentation and apparatus
Lattice dynamics
Materials research
Methods of structure determination
Neutron diffraction
Phase transitions
Powder diffraction
Resonance studies
Real and ideal crystals
Small angle scattering
Synchrotron radiation and applications
Symmetry and related topics
Techniques

STRUCTURAL STUDIES

Biological materials (proteins, viruses,
membranes, drugs, etc.)
Coordination compounds

Glasses and amorphous materials

Industrial materials

Inorganic and intermetallic compounds

Liquid crystals

Magnetic structures

Minerals

Organic compounds

Organo-metallic compounds

Polymeric materials

Surfaces, interfaces and films

A Workshop on the X-ray Powder-Diffraction
File is planned for 8 August 1984.

COMMITTEES

Organizing: Professor H. Saalfeld, Hamburg
Chairman

with the assistance of the
Gesellschaft Deutscher Chemiker

Programme: Professor U. Bonse, Dortmund
Chairman

ACCOMMODATION

Reservation will be arranged by a special travel
agency. A limited number of student dormito-
ries and camping facilities may be available.
Detailed information will be given in the second
circular.

FURTHER INFORMATION

A second circular with a call for papers, more
details of the programme, the general arrange-
ments and registration forms will be distributed
in the Autumn of 1983. Those wishing to
receive the second circular should return the
attached reply form or copies thereof to:

Gesellschaft Deutscher Chemiker
Abteilung Tagungen · Postfach 90 04 90
D-6000 Frankfurt/Main 90 F.R.G.

ASSOCIATED MEETINGS

At present the following meetings are
considered:

1. A Symposium on Neutron Scattering will
be held on 6-8 August 1984 at the Hahn-
Meitner-Institut, West-Berlin.
Organization: Prof. W. Saenger,
Institut für Kristallographie,
Freie Universität Berlin, 1000 Berlin 33, F.R.G.

Please return immediately, in any case before 30 June 1983.

Please use block letters and fill your address label below neatly so that it may be stuck directly on the envelope.

I am interested in attending the IUCr XIIIth Congress and General Assembly in Hamburg, 9 – 18 August 1984.

ADDRESS LABEL

(Title)	
_____	_____
(Initials)	(Name)

(Institution)	

(Street)	
_____	_____
(Zip)	(City)

(Country)	

Please send me the second circular yes ☐ no ☐

I hope to submit an abstract yes ☐ no ☐

I would be interested in using student accommodation yes ☐ no ☐

I would be interested in using camping facilities yes ☐ no ☐

I am interested primarily in topics: _____

Gesellschaft Deutscher Chemiker
Abteilung Tagungen
Postfach 90 04 90
D-6000 Frankfurt/Main 90
Federal Republic of Germany

Programme: Dr. M. S. Lehmann,
Institut Laue-Langevin,
Avenue des Martyrs, BP 156,
38042 Grenoble, FRANCE

2. An International Summer School on Crystallographic Computing is planned for 30 July – 8 August 1984 at the Max-Planck-Institut für Kohleforschung, Mülheim/Ruhr.
Organizing Committee:
Prof. H. Burzlaff, Prof. C. Krüger, Prof. G. Sheldrick;

Information: Prof. H. Burzlaff,
Institut für Angewandte Physik,
Universität Erlangen-Nürnberg,
Loewenichstraße 22, D-8520 Erlangen, F.R.G.

3. A Symposium on Small Angle Scattering and Related Methods will be held on 20 – 23 August 1984 at DESY, Hamburg.
Organization: Prof. H. Stührmann,
c/o EMBL, DESY, Notkestraße 85,
D-2000 Hamburg 52, F.R.G.
(together with Prof. P. W. Schmidt,
Columbia Mo., USA).

4. A Symposium on Metals and Intermetallic Compounds is planned for 20 – 24 August 1984 at the Technische Hochschule Aachen.
Information: Prof. W. Bronger,
Institut für Anorganische Chemie der
Technischen Hochschule Aachen,
Templergraben 55, D-5100 Aachen, F.R.G.

5. An International Summer School on Symmetry-Related Crystal Structures: Group-Subgroup Relations is planned for 20 – 24 August 1984.
Location: In the western region of the Federal Republic of Germany.
For further information write to
Prof. W. E. Klee, Institut für Kristallographie der Universität,
Postfach 63 80, D-7500 Karlsruhe, F.R.G.

The Schweizerische Gesellschaft für Kristallographie has announced to hold the "Paul Niggli-Symposium über geometrische Kristallographie und ihre morphologisch-stereochemischen Anwendungen" on 6 – 7 August 1984 in Zürich. Further information can be obtained from Prof. W. Nowacki,
Mineralogisch-Petrographisches Institut der Universität,
Balzerstrasse 1,
CH-3012 Bern, SWITZERLAND

FORMATION OF THE BRITISH CRYSTALLOGRAPHIC ASSOCIATION

The following note by Professor D.M. Blow, Chairman of the UK National Committee for Crystallography, recently appeared in The Royal Society News (reprinted in J. Appl. Cryst. 15, 577):

For many years the organisation of crystallography at a national level in the UK has been split between a number of scientific societies. The two largest groups are the Crystallography Group of the Institute of Physics and the Chemical Crystallography Group of the Royal Society of Chemistry, but a number of other societies cover crystallographic aspects of metallurgy, materials science, geology and biophysics. The UK Crystallographic Council provided a loose link between groups of crystallographers but it could not provide a speedy, collective response of UK crystallographers on, for instance, draft Health and Safety Executive legislation or EEC directives. Nor did its structure allow it to undertake activities with financial responsibilities, such as the organisation of a European Crystallographic Meeting in the UK.

The British National Committee for Crystallography, in addition to its duties as corresponding body to the International Union of Crystallography, provided a forum where matters concerning crystallography in the UK could be discussed. But it was not appropriate for it to deal with internal national matters. On the initiative of the National Committee, a working party was set up with the aim of establishing a new independent body covering all areas of crystallographic interest, to present the views of crystallographers collectively, to organise meetings of a crystallographic nature and to act as a centre for the dissemination of information on crystallography both within the profession and to a wider audience.

This initiative gained strong support. Particular help was given by the committees of the two largest groups in devising a system for incorporating their activities into the new Association. The British Crystallographic Association was inaugurated on 5 April 1982 at a meeting in Durham. The elected Officers of the new body are: President: Sir David Phillips, Professor of Molecular Biophysics in the University of Oxford and Biological Secretary, Royal Society; Vice-President: Professor Dorothy M. Hodgkin, Emeritus Professor in the University of Oxford; Treasurer: Professor C. A. Taylor, Professor of Physics at University College, Cardiff, in the University of Wales; Secretary: Dr A. C. Skapski, lecturer in physical chemistry at the Imperial College of Science and Technology, London.

THE SYMMETRY SOCIETY

Anyone interested in the activities of the Symmetry Society should contact Mike Stanford (Chairman) Crystallography Department, Birkbeck College, Malet St., London WC1E 7HX, Great Britain.

Besides the inherent beauty of symmetry, the Society is interested in the fun and fascination of the subject. Past speakers at meetings have been Dr David Singmaster on Rubik's Magic Cube and Prof. Stewart Robertson on Symmetry Classification of Convex Polyhedra.

ERRORS IN ERROR ANALYSIS

The following item was lifted from the Program and Abstracts of the ACA Summer Meeting at La Jolla, California, August 15-19, 1982. If at least one of the points does not strike a guilty chord then you probably haven't ever refined or reported a crystal structure!

11 ERRORS IN ERROR ANALYSIS AS PRACTICED BY CRYSTALLOGRAPHERS. A DIARY OF COMPLAINTS, DOUBTS, AND PROPOSITIONS. Verner Schomaker, Department of Chemistry, BG-10, University of Washington, Seattle, Washington 98195.

The original sin of chemical x-ray crystallographers is to work assiduously to reduce R , usually while proclaiming its unimportance, without knowing enough about items that determine the accuracy of their results. We refine on F instead of F^2 , following obsolete practices in regard to 'less than's', inserting perhaps with ultimate reason scandalously unrealistic values for the instability constant; rejoice over low values of the goodness of fit (whereas a low value of GOF usually only means that the acknowledged random errors are unusually large, whether genuinely so or

not); often retain data that are in gross error in consequence of a mistaken conviction that to reject such data is morally wrong; ignore covariances in reporting the esd's of derived quantities (e.g., bond lengths and bond angles); proceed in ignorance of how hydrogen atoms (or hopelessly disordered groups of atoms) need to be disposed of so that the other atom positions can be accurately assessed; apply elaborate tests to make fine distinctions between two alternative models when the overwhelming formal statistical conclusion has to be that both are exceedingly improbable; assume, hopefully or even fatuously, that to multiply the *a priori* s.d.'s of our results by the GOF is a sufficient act of caution; etc.

Points to be made: negative net intensities should be included in structure refinements. (The obvious way is formally correct.) The case that different hkl's suffer different intensity changes on radiation. The meanings of R , R_w , and GOF.

CHINA EXCHANGE AGREEMENT

The following notice has been received from P.D. O'Connor, Assistant Secretary, International Relations, Australian Academy of Sciences:

Applications are invited from scientists wishing to participate in the 1983/84 Australian Academy of Science - Academia Sinica scientific exchange program.

Intending applicants should have a specific program or project in mind, preferably one that has been developed in consultation with the institutes they wish to visit. Documentary evidence of Chinese interest and support will greatly strengthen the application.

Applications may be made for short visits (3 to 4 weeks) or for a longer term to carry out research projects or field studies. Preference will be given to proposals for visits designed to deal with topics in some detail, although proposals with broader objectives are not excluded, particularly where exploratory visits have not yet taken place.

In making its selections the Academy will be influenced by the following considerations:

- a. any special features of the proposal which make it logical for it to be carried out in China rather than in some other country;
- b. its scientific merit;
- c. the potential for developing further collaboration;
- d. the interest it is likely to arouse amongst scientists in similar fields of research in Australia, and
- e. evidence of support for the proposal from within China.

It should be noted that problems, and delays, may arise in arranging visits to institutes not under the control of Academia Sinica. Applicants should therefore concentrate on programs in which Academia Sinica has a direct interest.

Under the terms of the agreement travel expenses to China are Australia's responsibility and expenses within China the responsibility of Academia Sinica. No stipends or allowances are paid, nor provision made for return hospitality to Chinese hosts.

Application forms and a list of the Institutes of Academia Sinica are available from the Australian Academy of Science, P.O. Box 783, Canberra City, ACT 2601. For visits in the 1983/84 financial year early application is requested, as a considerable lead time is required.

Colin Kennard (Univ. Queensland) has just completed a visit of this kind to China and his report on same appeared in Chemistry in Australia 50, 18, 1982.

CRYSTAL DATA IDENTIFICATION FILE

In cooperation with the National Bureau of Standards, the JCPDS announces the availability of the NBS Crystal Data Identification File. This data base is a collection of data from the published literature which has been evaluated by the NBS Crystal Data Centre and cooperating data centres with the support of the Office of Standard Reference Data.

The result is a magnetic tape which permits the user to rapidly identify unknown crystalline materials using X-ray diffractometer measurements. For further details and leasing information, contact the JCPDS - International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081, USA.

NEW BOOKS

Members may find some of the following new releases of interest in their research/recreation:

Bacon, G. E.: The Architecture of Solids. 1981 = no. 58 of Wykeham Science Series.	paper \$ 16.50	US
Barrer, R. M.: Hydrothermal Chemistry of Zeolites. 1982.	57.50	
Brown, H. et. al.: Crystallographic Groups of Four-Dimensional Space. 1978.	80.95	
Dodson et al.: Structural Studies on Molecules of Biological Interest. 1981.	old price 98.00 new price 39.00	
Donohue, J.: The Structure of the Elements. 1974 Repr. 1982.	29.50	
Griffin, J.: Molecular Structure and Biological Activity, 1982.	75.00	
Harrison, W.: Electronic Structure and the properties of Solids. The Physics of the Chemical Bond. 1980. Instructor's guide + solutions manual, 1980	34.95 paper 3.50	
Holden, A.: Crystal + Crystal Growing. 1982	7.95	
Hutkins, D.: X-ray Diffraction by Disordered and Ordered Systems. 1981.	paper 28.75	
Luger, P.: Modern X-ray Analysis on Single Crystals. 1980.	53.50	
Nucleic Acids and Nucleoproteins. 1947, Repr. 1982 = Cold Spring Harbor Symposia on Quantitative Biology, vol. 12.	27.00	
Dobler, M. - Ionophores & Their Structures	(1981) \$57.50	
Fermi/Perutz (Eds.) - Atlas of Molecular Structures in Biology: V.2-Hemoglobin & Myoglobin	(1981) 45.00	
Fox, R. F. - Biological Energy Transduction: The Ureoboros	(1982) 32.95	
Glusker, J. P. (Ed.) - Structural Crystallography in Chemistry & Biology	(1981) 50.00	
Jenkins/Gould/Gedcke - Quantitative X-ray Spectrometry	(1981) 59.50	
McPherson, A. - Preparation & Analysis of Protein Crystals	(1982) 50.00	
Neidle, S. (Ed.) - Topics in Nucleic Acid Structure	(1981) 59.95	
Prince, E. - Mathematical Techniques in Crystallography and Materials Science	(1982) 22.50	
Sands, D. E. - Vectors & Tensors in Crystallography	(1982) 26.50	
Sayre, D. (Ed.) - Computational Crystallography	(1982) 34.50	
Vainshtein, B. K. - Modern Crystallography I, Symmetry of Crystals, Methods of Structural Crystallography	(1981) 47.50	
Windsor, C. G. - Pulsed Neutron Scattering	(1981) 85.00	

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

Volume A: Space-Group Symmetry edited by Th. Hahn, Institut für
Kristallographie, RWTH, Aachen, F.R.G.

1982, approx. 832 pp.

Cloth Dfl. 385,-/US \$165.00/£ 80.00 ISBN 90-277-1445-2

Individuals are entitled to purchase this volume at the reduced price of
Dfl. 215,-/US \$90.00/£ 45.00. They should declare that the copy is for their
personal use only and will not be put at the disposal of any library.

Crystallographic Statistics: Progress and Problems. Edited by S. Ramasesham, M. F. Richardson and A. J. C. Wilson. Pp. iv + 313. Bangalore: Indian Academy of Sciences.

Silinish, E. A.: Organic Molecular Crystals. Their Electronic States. 1980.	54.50
Smith, J. M.: Geometrical and Structural Crystallography, vol. 1. 1982.	29.95
Taylor, C. A.: A Unified View of Diffraction and Image Formation. * Wykeham Science Series no. 46, 1978.	paper 14.50
Teo, B. K.: EXAFS Spectroscopy: Techniques + Applications. 1981.	32.50
Todosiu, C.: Elastic Models Crystal Defects. 1982.	paper 27.00
Verma, A. R.: Crystallography for Solid State Physics. 1982.	24.95
Watson, J.: The DNA Story. 1981.	27.50
Whittaker, E.: Crystallography: An Introduction for Earth Science (and other Solid State) Students. 1981.	paper 19.95 hardbd 32.50
Winick, H.: Synchrotron Radiation Research. 1980.	65.00

To be published in October 1982:

Kleman, M.: Points, Lines & Walls: In Anisotropic Fluids & Crystalline Solids. 1982.	56.95
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To be published in December 1982:

Hazen, R.: Comparative Crystal Chemistry: Temperature, Pressure, Composition and the Variation of Crystal Structure. 1982.	41.95
Famplin, B. ed.: Inorganic Biological Crystal Growth. 1982.	60.00

POSITION SENSITIVE DETECTORS

Technology for Energy Corporation have recently released a new catalogue describing their range of Position Sensitive Proportional Counters for use with X-rays and neutrons. (Note that there will be a full session devoted to area detectors at CRYSTAL 14 in August this year).

Details of the following products are described:

Model 205 PSPC	X-ray detector
	Resolution: 50 μ m fwhm
	Anode: carbon coated quartz fibre
	Length: 5 cm
Model 210 PSPC	X-ray detector
	Resolution: 350 μ m fwhm
	Anode: stainless steel wire
	Length: 10 cm
Model 230 PSPC	Neutron detector
	Resolution: 3.3 mm fwhm
	Efficiency: 90% for 4Å neutrons

Model 375 Linear Position Sensitive Detector calibration masks.

Model 425N/X Two dimensional PSPC for X-rays and neutrons.

Model 465 Two dimensional PSPC for neutrons.

Model 200 Analog electronics for I-D PSPC.

Model 400 Analog electronics for 2-D PSPC.

Model 801 Analog Position Decoding Electronics.

Model 811 5-KV High Voltage Power Supply.

Model 831 Dual Parameter Input Buffer.

Model 841 Data Formatter.

If you are interested in receiving a copy of the new manual, please complete the form below and send to:

Quentron Optics Pty Limited
P.O. Box 364
BOX HILL. Vic. 3128.
Telephone: (03) 890 0501.

NAME

ORGANIZATION

ADDRESS
.....

TELEPHONE NUMBER

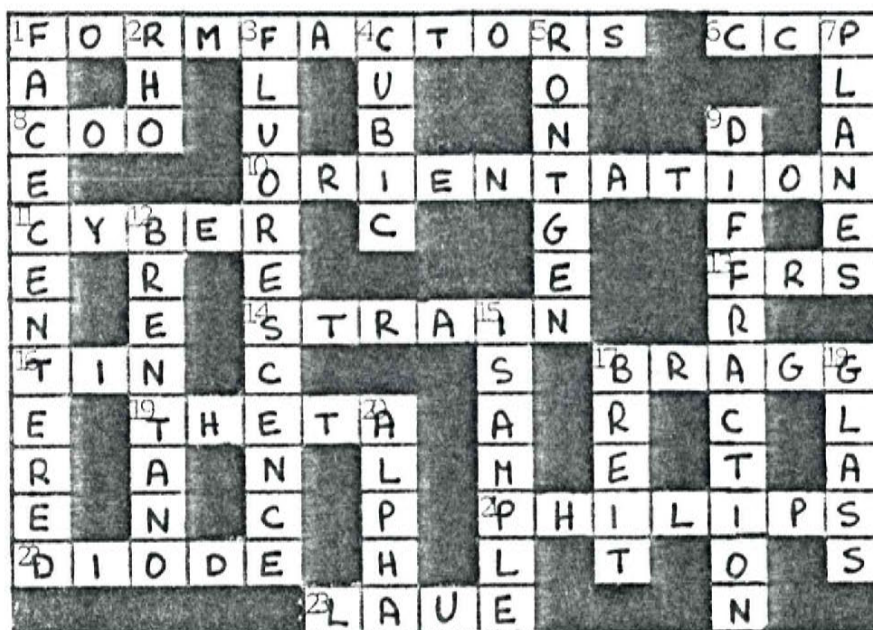
Please send me copy of new TEC manual.

Please place me on your mailing list.

My particular interest is

My requirement is	Immediate	Long Term
	6-12 months	File

CRYPTIC CRYSTALLOGRAPHIC CROSSWORD SOLUTION



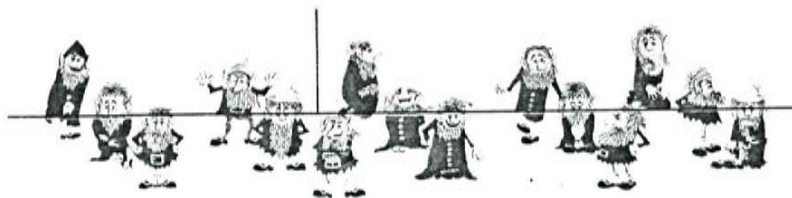
The first person to submit a (nearly) correct solution was Dr C.J. Howard of the AAEC at Lucas Heights. Well done Chris!

THE VANISHING LEPRECHAUN

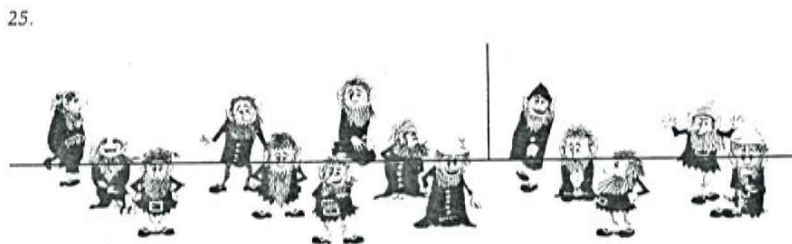
Ever had trouble locating that one last atom required to complete the complement in the asymmetric unit? Ever thought you had it, only to be disappointed when you calculated a difference Fourier?

Well here is a similar problem with a group of leprechauns - and you only have translational symmetry to worry about! Anyone who has the spare time to work out a solution and is first to send it to the Secretary will have their name immortalized in the next issue of the Newsletter.

25.
The Disappearing
Leprechaun, courtesy
William Elliot
Company, Toronto.
Arranged in this
manner, 15 leprechauns
are present.



26.
The Disappearing
Leprechaun, courtesy
William Elliot
Company, Toronto.
By rearranging the top
two pieces, one
leprechaun has
vanished. Which one?
Where has he gone?



SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

APPLICATION FOR MEMBERSHIP

Name:

Please print full name and include formal title (Mr, Ms, Dr, Prof., etc)

..... Title Forenames and/or initials Surname

Mailing address:

.....

.....

..... Postcode

Membership category:

☐ Regular. Annual
dues \$10

☐ Student. Annual
dues \$2

☐ Corporate. Annual
dues \$100

Membership is on a calendar year basis. Applications received after June 30 will apply for the following year unless otherwise requested.

Sponsorship:

Two current members of the Society must sponsor the application.
Please write to the Secretary if you do not know any current members.

Sponsor 1

Sponsor 2

Name (please print)

Signature

P.T.O.

Students must fill out the information below and have it certified by a faculty member of their school:

The applicant is known to me and is a bona fide student at
..... for the current academic year.
name of school

Faculty member:
Name Signature

Special interests:

Please indicate major fields of interest

Students should indicate the degrees or diplomas sought

1.
2.

Payment:

I enclose \$..... for membership dues for the year

.....
Signature Date

Please make cheques payable to the "SCA" and forward to:

Dr M.F. Mackay
Department of Physical Chemistry
LaTrobe University
BUNDOORA, VIC. 3083