Society of Crystallographers

in

Australia

Newsletter No. 8

March 1984

Contents:

In recent years most of Chris' effort has been in developing the high resolution neutron powder diffractometer at HIFAR. In Europe he will participate in similar work at the Institut Laue-Langevin in Grenoble, although for the most part he will be based in Edinburgh. Chris also hopes to visit the Rutherford-Appleton Laboratory, where a spallatron neutron source may be nearing completion. His Visiting Fellowship will also enable him to use the time-of-flight powder diffractometers associated with the pulsed neutron source at the Argonne National Laboratory (USA) and possibly the X-ray powder diffractron facility at the UK's Daresbury synchrotron radiation source.

While in Europe Chris will attend the 13th Congress and General Assembly of the International Union of Crystallography to be held in Hamburg FRG 9-18 August 1984, and the Symposium on Neutron Scattering in West Berlin which precedes it (6-8 August).

14TH I.U.Cr. CONGRESS - PERTH, 1987

The Organizing Committee for the Perth I.U.Cr Congress reports that arrangements for the Congress are now well advanced. The dates selected (14-20 August) are relatively firm although they have not yet been approved officially by the I.U.Cr.

The recent Australia-wide competition for a Congress logo produced more than 20 submissions, from which the entry reproduced below was selected as the winner. This logo will be used on all official Congress correspondence, on posters and pamphlets for distribution at Hamburg, and on T-shirts to be used for further publicity. An order form for the T-shirt is enclosed below.

Syd Hall would like to have a snappy slogan on the back of the T-shirt - something akin to:

"Something to BRAGG about" or

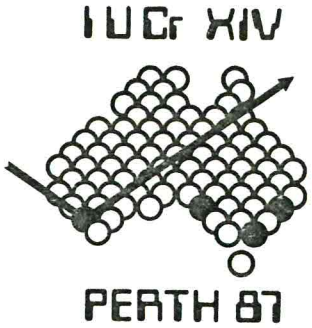
'DOWNUNDER, where x becomes $\bar{x}$!".

Please send your order form and slogan suggestions to Syd Hall (Univ. WA, Crystallography Centre) NOW - we need to present a high profile both at home and overseas in order to make the Perth meeting a real success (see the President's message below).

XIVth INTERNATIONAL CONGRESS AND GENERAL ASSEMBLY
INTERNATIONAL UNION OF CRYSTALLOGRAPHY
PERTH, AUSTRALIA AUGUST 14-20, 1987.

Local Chairman
Dr. E.N. Maslen
Crystallography Centre
U. Western Australia
Perth 6009, AUSTRALIA.
Ph: 380 2727 Tx: 92992

Programme Chairman
Prof. H.C. Freeman
Dept. Inorganic Chemistry
University of Sydney
Sydney 2006, AUSTRALIA
Ph: 660 0522 Tx: ******



LOGO DESCRIPTION

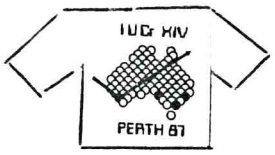
The logo for the XIVth Congress of the International Union of Crystallography shows the host country, Australia, as a layer of spheres. These represent a plane of close-packed atoms in a crystal lattice. A ray is reflected from the sphere located at the host city of Perth. This represents a reflection or diffraction of particles (usually X-rays, electrons or neutrons) from a crystal plane; a technique commonly used in the crystallographic study of atoms in solids.

This logo has added significance for Australia since the Nobel Laureate W.H. Bragg who lived and worked in Adelaide 1886-1909, discovered the law describing the diffraction of particles from a crystal plane. His son W.L. Bragg, also a famous crystallographer and Nobel Laureate, recieved his early schooling in Australia.

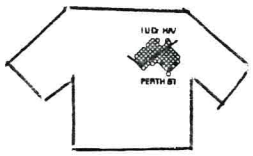
The dark spheres in the logo highlight the locality of the host city of the Congress, and focus on the sites of pre- and post-Congress meetings at Sydney, Melbourne and Adelaide.

WINNER OF THE LOGO COMPETITION

The logo of Associate Professor David L. Kepert of the University of Western Australia was selected by the Local Organizing Committee as the winning entry. Dr. Kepert, who is a coordination chemist in the Department of Inorganic and Physical Chemistry, recieved the prize of $150. donated by the Chamber of Mines of Western Australia. The final form of the logo (as shown) was prepared by the Media Services Unit of the University of Western Australia.



ORDER FORM : CONGRESS SHIRTS



Name: .....

Address: .....

Shirt Style

1. Gold T-shirt ($6.50)
2. Gold shirt with green collar ($9.00)
3. Gold windcheater ($14.00)

Logo

A. large frontal
B. small left chest

Shirt Sizes

SM, M, L, OS

Slogan (on back)

a. To be decided (see newsletter)
b. No slogan

Number	Style	Size	Logo	Slogan	Cost
				TOTAL	

Make cheque to: "IUCr CONGRESS PERTH"

Send to: Crystallography Centre, University of Western Australia, Nedlands 6009, Western Australia.

(Delivery within 30 days)

PRESIDENT'S MESSAGE

While it is always desirable that Australian crystallographers attend Congresses of the International Union, the meeting in Hamburg has special significance. It is the Congress preceeding our meeting in 1987. As many Australians as possible should attend to convince our colleagues that the journey to Australia is professionally and socially worthwhile.

At the present level of international exchange rates Europe is cheaper for Australians than it has been for many years. I do not think that two weeks in Hamburg would be any more expensive than the same period at any place in Australia involving the use of our "fiercely competitive" internal airlines.

T.M. Sabine

SATELLITE MEETINGS FOR THE PERTH CONGRESS

It is desirable that satellite meetings to the 1987 Congress be publicised at the 1984 Congress. For this to be done certain formalities are required by the International Union of Crystallography. These formalities should be attended to immediately. Would those groups contemplating organising satellite meetings please contact Hans Freeman on (02) 692 2757 (Univ.) or (02) 328 6859 (home) to receive the appropriate forms.

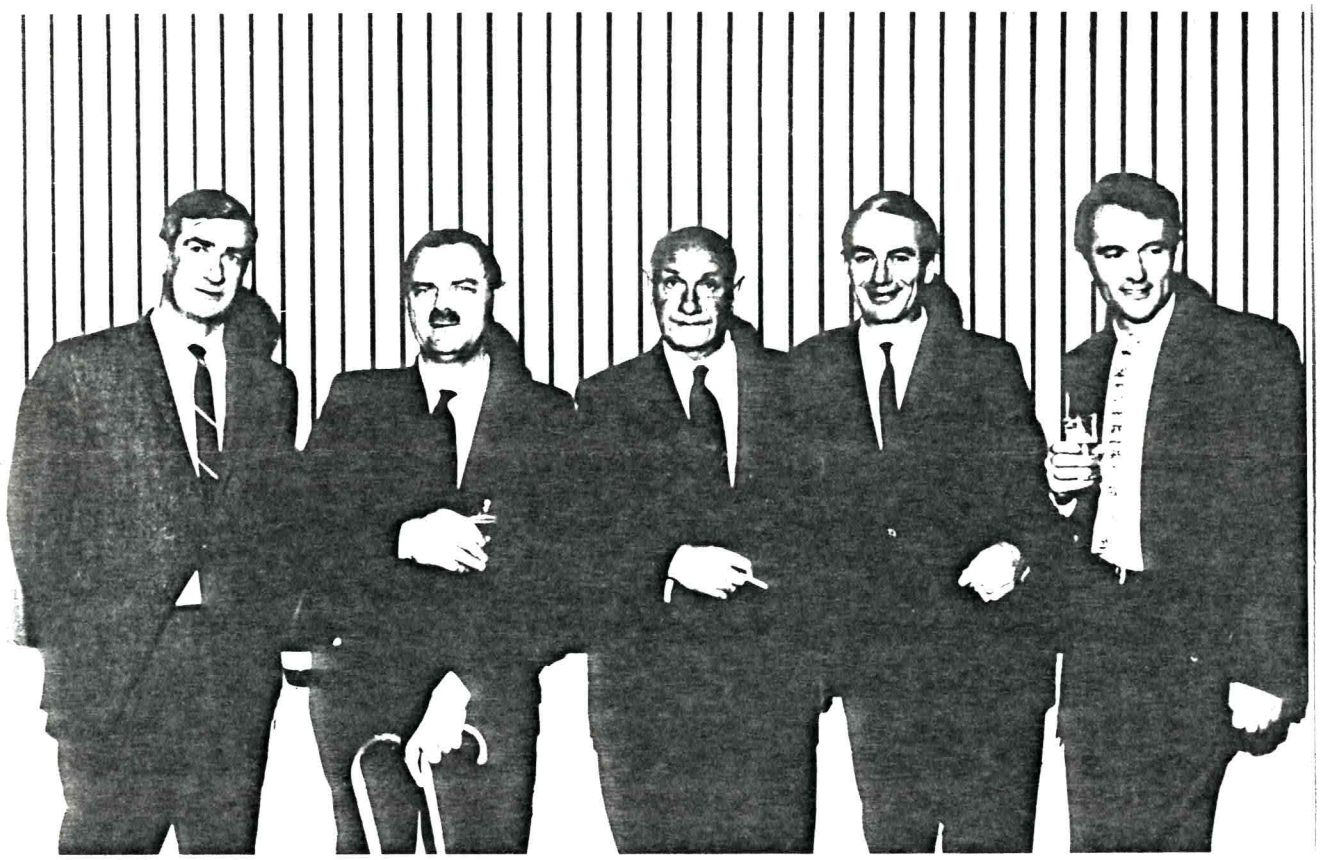
PREVIOUS MEETINGS OF THE SCA

The Secretary extends his thanks to Ted Radoslovich, Frank Moore, Hans Freeman, Jeff Wunderlich, and Bryan Gatehouse for their information about the venues, dates and Organizing Committees of previous meetings of the Society. The new updated list appears below. Note that there is still only very sketchy information about the 2nd, 3rd and 4th meetings. Also, the terminology "CRYSTAL 15" etc. was initiated by Ted Radoslovich while he was organizing the Adelaide meeting in 1971 - before the SCA was formed. Please let the Secretary know if you have any further details to add to the list.

Meeting	Year	Date	Venue	Organizing Committee
15	1985	May	Adelaide	M.R. Taylor
14	1983	Aug 30-Sept 2	Morpeth, NSW	H.R. Tietze, K. Colyvas
13	1982	Feb 2-5	Univ. Qld	C.H.L. Kennard, G. Smith
12	1980	Jan 30-Feb 2	ANU	G.M. McLaughlin, P.A. Tucker, T.R. Welberry
11	1978	Jan 29-Feb 2	Bendigo	B.M. Gatehouse, D. Lloyd I.E. Grey, L.A. Bursill

10	1976	Feb 12-15	Hawkesbury Agr. Col, Camden, NSW	F.H. Moore, N.C. Stephenson H.C. Freeman
9	1973	Feb 14-16	LaTrobe Univ.	M.F. Mackay, D.A. Wright, J.A. Wunderlich
8	1971	Aug 18-20	Adelaide Univ.	E.W. Radoslovich, M.R. Snow J.B. Jones, M.R. Taylor
7	1970	Feb 12,13	Univ. NSW	N.C. Stephenson, J. McConnell
6	1968	Aug 21-23	Univ. WA	E.N. Maslen, J. Graham
5	1967	Aug 17,18	Monash Univ.	B.M. Gatehouse, H.C. Bolton
4	1964		Melbourne Univ.	
3	1963		Lucas Heights	
2	1962			
1	1961	May 25,26	Univ. Sydney	H.C. Freeman

OLD PHOTOGRAPHS



The above photograph was taken from an original recently loaned to the Editor by Jeff Wunderlich. For the younger readers the gentlemen shown are (from the left): W.D. (Dave) Wadsley (dec. 6.1.1969), A.M. (Sandy) Mathieson, J. Fridrichsons, B. Dawson (dec. 20.2.1975), and J.A. Wunderlich. It was taken in 1966.

This photograph is an irresplacable piece of the history of Crystallography in Australia. Many more examples of its kind must be hiding away in the closets and personal papers of many of the readers of this Newsletter, only to be eventually lost or accidentally destroyed. With this in mind the Secretary extends an invitation (plea) to anyone who possesses a photograph which could be of relevance to the development of Crystallography in Australia, especially if it involves the Crystallographers themselves, to forward said photograph to him for copying and immediate return. The copy will be placed in a file of documents which will be transferred to the holder of the office of Secretary at each SCA election. This file could ultimately constitute a central repository for all forms of historical material relating to Australian Crystallography, but in the first instance the Secretary is keen to obtain group photographs taken at Crystal meetings. Please help if you can.

NATIONAL COMMITTEE FOR CRYSTALLOGRAPHY

For those readers who have wondered what, or who, is the National Committee for Crystallography of the Australian Academy of Science, the membership of said body is as follows (effective from April 1, 1984):

H.C. Freeman (Chairman: term expires 1/4/87)
E.N. Maslen (1/4/87)
J. Stonehouse (1/4/87)
R.L. Segall (1/4/86)
T.R. Hicks (1/4/85)
T.M. Sabine (ex-officio SCA representative)

This committee, not the SCA, is the official body which advises the Academy of Science on all matters relating to Crystallography in Australia. The members serve terms of three years, at the end of which period new members are nominated by the current committee. There are no elections held (except by the 6 members for their own chairman), although the Academy has the ability to veto the slate of nominations proposed by the Committee. In fact, the first three members named above (to replace A.F. Moodie, I.E. Grey and M.R. Snow) have yet to be ratified by the Academy. Meetings of the Committee can be called at any time (and can be financed by the Academy), but they have tended to be few and far between in recent years. The only formal input to the decision making process available to the SCA is through its one and only ex-officio member, who is the SCA President of the day.

The National Committee for Crystallography did, of course, exist long before the SCA was formed (1977) but there is no question of the fact that the SCA handles all of the grass-roots crystallographic activities in Australia at the present time. Moreover, the SCA, unlike

the Academy (and hence the National Committee), has assumed through its Temporary Standing Committees financial and organizational responsibility for the Crystal meetings and the forthcoming I.U.Cr. Congress in Perth. In effect, therefore, the National Committee plays a role largely in funnelling official information through to the Academy.

On the assumption that both bodies will (and must) continue to exist, it may be worth considering the implementation of closer official ties between the SCA and the National Committee, not only to avoid duplication of effort, but also to ensure that a united and representative opinion from the Crystallography community in Australia is presented to the Academy.

The Editor invites the readership to submit further comment on this issue.

REPORT ON THE 1983 RACI SOLID STATE DIVISION SYMPOSIUM

A two-day symposium organized by Hans Jaeger and Rod Hill on behalf of the Solid State Division of the Royal Australian Chemical Institute was held at the Victorian College of Pharmacy, Parkville, Victoria, on November 24 and 25, 1983. Some 80 persons attended about 50 oral and poster presentations devoted to the bulk properties of solids, concentrated into the first day of the meeting, and the properties of surfaces and catalytic technology, concentrated into the second day. The following is a summary of the material devoted to bulk properties.

The first Session began with Opening Remarks by Prof. Dan Haneman (Chairman of the Solid State Division). Dr Ian Grey (CSIRO Division of Mineral Chemistry) then presented his Plenary Lecture on the Structural and Solid State Chemistry of Oxides and Minerals, particularly those showing Order/Disorder Phenomena. This lecture gave a fascinating account of the brilliant combination of applied and fundamental solid state chemical principles in the solution of complex problems in process chemistry. It represented a small part of the research for which Ian was awarded the inaugural 1982 RACI Solid State Division Medal at 7NC in Canberra last year. The Session was concluded with a very thought provoking invited talk by Prof. Bruce Hyde (RSC, Australian National University) on the Role of Stoichiometry in Determining the Structure and Stability of Inorganic Solids.

The second Session began with two presentations on the application of high resolution imaging and convergent beam electron diffraction in solid state chemistry. The next three papers described new techniques and applications of X-ray and neutron powder diffraction, with particular emphasis being placed on their roles in the study of natural and synthetic zeolites. The final two talks continued this zeolite theme by presenting new data on the structure of pentasil zeolites and problems with the interpretation of high resolution NMR spectra of silicalite.

The after-lunch Session commenced with a fascinating and very welcome Plenary Lecture by Prof. Judge Bevan (School of Physical Sciences, Flinders University) on the Crystal Chemistry of Anion Deficient Fluorite Related Structures. The talk was punctuated

throughout by the appearance of a seemingly endless supply of superb polyhedral models from a host of cleverly concealed cardboard boxes under and around the dais at the front of the theatre. Together with Prof. Bevan's narrative they provided colourful and concise insight into the very complex crystal chemistry of this system. The next three talks described studies of the crystal chemistry of the hydrides of Mg_5Si_3 alloys, phases in the Bi_2O_3-PbO system, and the mobility of anion vacancies in alkali halides. The final talk was a very entertaining and topical account of recent structural studies on technetium radio-pharmaceuticals.

The fourth Session began with Plenary Lectures by Drs Henry Rossell and Mike Swain (CSIRO Division of Materials Science) on the Structure and Development of Partially Stabilized Zirconia. Dr Rossell presented an explanation for the superior thermo-mechanical properties of Mg-PSZ using a series of superb observed and calculated electron diffraction micrographs rationalized in terms of crystal chemical principles in the fluorite related superstructure phases at the interface between the matrix and the precipitates. Dr Swain documented changes in the mechanical properties of PSZ and zirconia-containing ceramics through transformation toughening, and related these improvements to the processes of volume dilation and shear strain developed at the tips of incipient cracks. The last three talks in this session were very entertaining presentations of a more Industrial nature devoted to the subjects of wood fibre substitutes for asbestos in cement sheeting, an overview of the current and future problems in the commercial utilization of phosphogypsum, and the development of a new method of mineral modal analysis in the SEM.

Rod Hill

INTERNATIONAL SUMMER SCHOOL ON CRYSTALLOGRAPHIC COMPUTING

The 1983 International Summer School on Crystallographic Computing was held at Kyoto, Japan from 18-26 August. The school was organized by the IUCr Commission on Crystallographic Computing and the Crystallographic Society of Japan, run under the auspices of the IUCr and ICSU, and sponsored by a large number of professional and commercial bodies.

This was the first IUCr computer school to be held in the Asian/Pacific area and the second not to be run independently from an IUCr Congress (the first was in Bangalore in 1980). The lecture program covered a broad range of crystallographic applications, most with a strong macromolecular flavour. Major topics included data measurement and error treatment, solution methodology (direct and indirect), software packages and data-bases, refinement and phase extension, computer graphics, powder analysis, precision electron density studies and electron diffraction.

The program structure placed particular emphasis on the use of work sessions. The approximately 30 lectures were given in the mornings leaving most afternoons for parallel 90-minute work periods. These were limited to groups of 10-20 participants. Since English was not the first language of most participants these sessions were of particular importance. The work sessions proved to be the real kernel of the school and level of effort input by both lecturers and participants ensured their success. Language considerations also necessitated a particularly high level of lecture presentation and documentation. This is reflected in the detailed lecture notes which are due to be published as a book early next year.

Topics of special interest at the school were the use of maximum entropy for protein phase extension techniques by Gerard Bricogne, and an excellent description of electrostatic potential calculations by Mark Spackman. The importance of precision density studies to protein work was also impressively demonstrated by Noriyoshi Sakabi in his study of 2Zn insulin. Recent advances in array processors and graphics hardware was also very well covered by Bill Furey and Jim Pflugrath. For the more established applications, the instruction of Bill Clegg, Henk Schenk, John Rollett, Joel Sussmann and Peter Murray-Rust was especially appreciated.

With over 150 participants and 30 lecturers from 15 different countries, the school organization involved considerable local support. Tamaichi Ashida and his local committee did a truly excellent job. Participants were housed at two hotels within walking distance of each other and these also served as the lecture venues. Unfortunately the opening mixer was under-attended due to a typhoon that left many participants and lecturers stranded all over Japan. However, with an effiency that characterised the running of the whole school, our hosts worked through the night to ensure that all made the first day. On the social side, a day trip to the ancient capital of Nara and a half-day visit to the Institute of Protein Research in Osaka were welcome breaks to a full school program. The social highlight of the school was a splendid banquet.

In summary, the school proved to be of real scientific benefit to participant and lecturer alike. It provided participants from Japan, China and Asian countries with the opportunity to receive tuition from authorities in a wide range of fields, and enabled lecturers to meet and exchange ideas with fellow crystallographers who often do not get to the usual scientific meetings. Congratulations are due to everyone - organizers, lecturers and participants - who made this a productive and enjoyable meeting.

Syd Hall

From the October 1983 ACA Newsletter.

FUTURE MEETINGS

- May 6-20, 1984: International School on Direct Methods of Solving Crystal Structures, Erice, Italy. Contact: Prof. L. Riva di Sanseveriono, Instituto di Mineralogia, Piazza di Porta San Donato 1, 40127 Bologna, Italy.

- May 14-18, 1984: The Horizons of Science, 54th ANZAAS Congress, ANU, Canberra. Contact: Congress Secretariat, Dulcie Stretten Associates, 70 Glenmore Road, Paddington, NSW 2021.

- May 21-25, 1984: American Crystallographic Association Spring Meeting. Lexington, Kentucky, U.S.A. Contact: Prof. D.E. Sands, Dept. of Chemistry, University of Kentucky, Lexington, Kentucky, 40506, U.S.A.

- July 30-Aug 8, 1984: International Summer School on Crystallographic Computing, Max-Planck-Institut fur Kohlenforschung, Mulheim, FRG. For application forms please contact: Dr S.R. Hall, Crystallography Centre, University of WA, Nedlands, W.A.

- Aug 9-18, 1984: I.U.Cr. 13th Congress, Hamburg, Germany. Contact: Gesellschaft Deutscher Chemiker, Abteilung Tagungen, Postfach 90 04 90, D-6000 Frankfurt/Main 90, Federal Republic of Germany.

- Aug 14-19, 1984: 8th European Congress on Electron Microscopy, Budapest. Contact: Congress Bureau Motesz, Budapest P.O. Box 32, H-1361 Hungary.

- Aug 27-31, 1984: Sixth National Congress, Australian Institute of Physics, Griffith University, Brisbane. Contact: Dr B.W. Thomas, Dept. of Physics, Queensland Inst. Techn., GPO Box 2434, Brisbane, Qld 4001.

- May, 1985:. Crystal XV, Adelaide. Contact: Dr M.R. Taylor, School of Physical Sciences, Flinders University, Bedford Park, South Australia.

- May 24-June 6, 1985: The determination and interpretation of small structural differences, Erice, Sicily. Contact: Prof. L. Riva di Sanseverino, Int. School of Crystallogr., Piazza Porta San Donato 1, 40127 Bologna, Italy.

INORGANIC CRYSTAL STRUCTURE DATA BANK-ICSD

The Editor wishes to correct a mistake in the last Newsletter relating to the cost for one year's use of the magnetic tape data base for Inorganic Crystal Structures. The fee is DM 2200 rather than DM 220 as previously stated.

David Hay (CSIRO Materials Science) and Tony Grattan (CILES) have expressed interest in obtaining a copy of the ICSD tape but have indicated that the rental would have to be shared among a number of users from different organizations. If you are interested in

contributing to the fee please contact David or Tony for further details, or write direct to Dr H. Behrens or Dr G. Ebel, Fachinformationszentrum, Energie, Physik, Mathematik GmbH, D-7514 Eggenstein-Leopoldshafen 2, Federal Republic of Germany.

ON THE PUBLISHING OF COORDINATES

In the last few years, publishing costs have risen sharply and many journals have attempted to reduce costs by depositing more and more data. In the case of crystal structure analysis, deposition of coordinates frequently means that these fundamental data are unavailable to most of the scientists who might otherwise use them. Most libraries do not carry the microform editions of the journals; the microforms are frequently illegible; the data banks do not respond to individual requests; and the availability of the data banks can not be counted on.

This is an appeal, which originates in our National Committee on Crystallography, to ACA members to help ensure that coordinates are published. In submitting your own papers to journals that do not ordinarily publish coordinates (such as JACS, Inorganic Chemistry, and J. Org. Chem.), you can provide a good quality glossy photo of a table of coordinates containing atom type, coordinates with estimated errors, and U eq. In refereeing papers, you can point out the importance of such information and recommend that the information be included in the paper in question.

The coordinates of a crystal structure analysis can be presented succinctly, and when this is done a wealth of other parameters, such as bond lengths, bond angles, non-bonded contact, hydrogen bonding, intramolecular forces, details of packing, etc. can be routinely derived. Thus the coordinates are a basic source for future science, and their inclusion or exclusion is important in determining the value of our activity in society.

D. Sayre

From the December 1983 ACA Newsletter.

CHINA EXCHANGE AGGREEMENT

Applications are invited from scientists wishing to participate in the 1984/85 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.

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.

Telephone inquiries may be directed to Ms Carrie Steffen (062) 48-6011.

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