

Society of Crystallographers in Australia



SCA

Newsletters

No 39, August 98

The SCA homepage is located at <http://www.sca.asn.au>

sca39

FROM THE PRESIDENT

Despite sheltering half way around the world, our newsletter editor was able to keep track of me using the power of the omnipresent Internet. I am presently spending six months study leave, previously "sabbatical" before the newspeak correctness got to it, in the laboratory of Joel Sussman at the Weizmann Institute of Science (WIS) in Israel. Joel is known to many of you as a protein crystallographer and is also the current head of the Brookhaven Protein Data Bank. This explains why after two weeks in Israel, I have yet to see him, since he is in the U.S.

First impressions of a country may of course be quite misleading but that is currently all I have to offer. If Joel's research group is anything to go by, this is truly a crossroads. There are Germans, Chileans, Americans, Italians and naturally a few Israelis. The WIS is superbly organised for the visitor. There is an office for visiting scientists that prearranges accommodation and all the other necessary paperwork – very nice for a stranger to a country and its language. Israel is a small country whose settlers in the 19th and early 20th century believed in a return to the land and agriculture of their forefathers more than 2000 years ago. This built a strong, modern agricultural industry, which still exists today but is rapidly declining in national importance. The country as a whole is "gambling" its future on high technology industries, largely computer based. This leads to a society in which doctors and lawyers are relatively poorly paid and esteemed whereas scientists and engineers are keenly sought after and well paid. While the average income of Israelis is well below that of Australians, their University professors are paid more with more generous benefits – dream on Australians!

The relatively small crystallographic community is expanding principally, as in most countries, by the boom in protein crystallography. From one group at the Weizmann, fifteen years ago, there are now groups at the Hebrew University in Jerusalem, at the Haifa Technion, and a new group is currently being established at Tel Aviv University. The small band of Israeli crystallographers is

now facing the reality of organising and hosting the 2002 IUCr meeting and Congress in Jerusalem.

As unlikely as it seems, given the present tensions and disagreements in the Middle East, there is an active proposal to establish a multinational synchrotron facility involving amongst others Jordanians, Palestinians, Egyptians, Saudi Arabians and Israelis. It would be nice if such a facility was constructed and synchrotron radiation could be a contributor to peace in the region.

I look forward to seeing you in Malaysia at AsCA meeting in October, Shalom,

Notice of SCA Business Meeting

A business meeting of the SCA will be held in conjunction with the Third Meeting of the Asian Crystallographic Association to be held in Bangi in the state of Selangor, Malaysia, from 13-15th October, 1998. The business meeting has been scheduled for 1-2 pm on Thursday, 15th October.

BUSINESS MEETING 13.00-14.00 15 October, 1998

PROPOSED AGENDA

- 1. Apologies**
- 2. Minutes of previous Business Meeting, April 4, 1997, Queenstown**
- 3. Business arising from the Minutes**
- 4. President's Report**
- 5. Treasurer's Report**
- 6. Report from the National Committee for Crystallography (including an update on access to synchrotron radiation)**
- 7. Reports on AsCA and IUCr meetings**
- 8. Date and venue for CRYSTAL XXI meeting**
- 9. Other Business**
- 10. Report from the Nominations Committee and transfer to new Council**

Trevor Hambley

Secretary SCA

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

St. Vincent's Institute of Medical Research

The Protein Crystallography Unit at St. Vincent's was founded by Dr Neil Isaacs in 1978. The establishment of the Unit at the Institute was a natural progression from its early strengths in protein chemistry and structure built up by the Institute's founding Director, Pehr Edman and subsequently continued by Frank Morgan and Jack Martin. Neil worked at St. Vincent's for nine years before accepting the offer of a new Chair of Protein Crystallography at the University of Glasgow, Scotland. Whilst at St. Vincent's, Neil solved the structure of a "goose-type" lysozyme

and crystallized human chorionic gonadotropin, a hormone involved in early pregnancy. He went on to solve the structure of the hormone in his new lab and the results were recently published in Nature.

The Protein Crystallography Unit was re-established in 1991 with the appointment of Michael Parker as Head of the Unit. The position was generously supported by a Senior Research Fellowship to Michael from the Wellcome Trust. A pressing requirement in the early years was the need to equip the Unit with state-of-the-art instrumentation. This was made possible through the enthusiastic support and efforts of the Deputy Director, Bruce Kemp, and the generous financial support of The BHP Community Trust, The Jack Brockhoff Foundation and The Ian Potter Foundation. In recognition of this support, the Unit was renamed as The Ian Potter Foundation Protein Crystallography Laboratory. The Laboratory is now well-equipped with a Rigaku RU-200 rotating anode generator, two MARresearch image plate detectors and associated cryocooling equipment from Oxford Cryosystems. The rapid pace in computer technology over the last decade has been reflected in the changes that have occurred in the lab. Neil's "mainframe" computer, a microVAX II, was replaced by a Digital VAX cluster in the early 90's, consisting of three workstations, which in turn is now gradually being replaced by a cluster of nine Silicon Graphics computer workstations. Computer Graphics facilities have evolved from Neil's Silicon Graphics Iris workstation to an Evans and Sutherland ESV3 workstation to the current Silicon Graphics Indigo 2 workstations.

The lab has been fortunate in attracting some very talented crystallography postdocs. over the years including Matthew Wilce, Bostjan Kobe and Jamie Rossjohn. Bostjan is in the process of setting up a second protein crystallography lab in the Institute. We have also been fortunate to have discovered the "crystallization goddess", Susanne Feil, who appears to have "green" fingers when it comes to growing protein crystals. The lab has concentrated in three major areas of biology over the last seven years: membrane-interacting proteins, detoxifying enzymes and protein kinases. Particular highlights include the structure determinations of aerolysin, perfringolysin O, twitchin kinase and various glutathione transferases. As the lab grows so will our interests into other areas of modern biology.

Michael Parker

REPORTS ON NEW DIFFRACTOMETERS

University of Canterbury

The University of Canterbury chemistry department upgraded a Siemens P4 diffractometer to a SMART CCD system at the beginning of May 1997. Since then we have adjusted to obtaining one new data set each night plus one during the day if the work load demanded it. We operate a fixed anode tube at 1800 watts and obtain results comparable with those previously obtained using the P4 in normal sequential bisecting mode. Higher power (3Kw) enables smaller crystals to be studied and, of course, all operations are enhanced by continuous low temperature operation.

Normal data sets take the same time regardless of cell size but much shorter times (one hour data collections) can give rough structures though this will never become our standard practice. I have also used a SMART CCD on the Daresbury synchrotron with spectacular success using extremely small crystals and short exposure times at those very high intensities.

Our SMART is heavily used for wood fibre diffraction determining the preferred orientation of cellulose crystallites in sawn timber and this industrial application has proved both interesting and lucrative. There are many fascinating potential applications in teaching powder diffraction in almost real time.

These instruments will put conventional sequential diffractometers into museums within 5 years and will, themselves, be replaced with new medical imaging technology within 5 years.

Ward Robinson

CRYSTAL FRAGMENTS

Syd Hall (University of Western Australia, WA) gave an invited lecture at a conference on 'Computers in Structural Chemistry and Molecular Biology' held from 16th-17th June in the Department of Chemistry, University of Manchester in conjunction with celebrations in Manchester to mark the 50th Anniversary of the First stored-Program Computer. Syd spoke about "Coping with the Structural Chemistry Information Explosion" Approximately 84 delegates from the UK, Europe and Australia heard speakers John Helliwell, Durward Cruickshank (UMIST), Frank Allen (Cambridge), Janet Thornton (London), Sir Thomas Blundell (Cambridge), Eleanor Dodson (York), Michael Woolfson (York), Alwyn Jones (Uppsala) and Tony Crowther (Cambridge).

Bee Gan (formerly Curtin Univ, WA) is now employed as a research scientist in the Microstructural Analysis Unit, Faculty of Science, at UTS. I took the position up in November of last year and are currently on a two year contract. My job is mainly to perform scientific research using characterization techniques in the Unit, namely X-ray diffraction, X-ray fluorescence and possibly some electron microscopy. Besides conducting research, I assist with the teaching of the above mentioned techniques to students and support postgraduate students in their projects.

Dr Stephen Holt has been appointed to one of the Australian Synchrotron Research Programs Fellowships,

The Project is entitled "Surfactant Mediated Crystallisation of Oriented Inorganic Phases at the Air-Water Interface." The project aims to investigate the relationship between organised surfactant systems and the crystallisation of inorganic phases at the solution film interface. This is being undertaken by studying Langmuir films and self assembled monolayers at the air-water interface with the appropriate subphase

NEW MACROMOLECULAR FACILITY

Two New Area-Detector Diffractometers for UWA

The two new area-detector diffractometers at the Crystallography Centre at the University of Western Australia were officially "blessed" on Wednesday July 29 with a gathering of the financial backers of the RIEFP grant and other funding sources. The BRUKER Smart1000 AXS has already collected 120 data sets and a MAR345 Image-plate system has been installed and tested. At this opening science-fest Syd Hall, Allan White, Victor Streltsov and Matthew Wilce espoused the future activities of the Centre in their respective areas.

This occasion was of special importance in that it marked the commencement of macromolecular structure studies at the Crystallography Centre and University. The need for this initiative has long been recognised at UWA but it took a 1995 university review recommendation to bring together the financial support for diffractometers and a protein crystallographer appointment. The appointment of Matthew Wilce, previously in the Department of Biochemistry at the University of Sydney, was made possible through support from the Raine Medical Foundation, the Crystallography Centre in the Faculty of Science, and the Department of Pharmacology in the Faculty of Medicine. Matthew heads up the macromolecular effort and holds a joint appointment with the Crystallography Centre, and in the Department of Pharmacology where he has facilities for bacterial expression, purification, and crystallisation. The MAR345 at the Centre is mounted on an existing RU-300 generator and has focus mirror optics with an Oxford cryo-cooling stage. The Centre has also recently installed four new Digital 600au Alpha work-stations with Powerstorm 51T graphics accelerators. Dr Aaron Oakley has also joined the macromolecular effort after winning a University Post Doctoral Fellowship held jointly with Pharmacology and Crystallography. Matthew's macromolecular group will be studying an integral membrane protein - mechano-sensitive channel protein, protein/DNA complexes and complexes of subunits of ATPase (with Dr. Andrew Rodgers).

AsCA'98 UPDATE

In June of this year I was fortunate to be able to visit Bangi and spend two weeks at the Universiti Kebangsaan during a recent trip to Malaysia. I was delighted to find that preparations for AsCA'98 are well advanced. I was also able to visit the conference venue, an excellent modern hotel with fine facilities. The areas set aside for the three lecture sessions seem entirely adequate and the lecture rooms open onto the poster area, which in turn, is adjacent to the area set aside for the trades exhibitors. I sampled some of the fine food available in the three restaurants in the hotel. They will, I am sure, cater more than adequately for the requirements of all participants.

During my visit, I attended a meeting of the Local Organising Committee and was able to hear at first hand that their planning for the meeting is well advanced and that they are strongly committed to making AsCA'98 a memorable experience for all participants. I also saw the accommodation arranged for participants preferring hostel rooms. The Kamsis Abu Zain is a modern hostel with good facilities. Transport to and from the Hotel Equatorial has been arranged for participants staying at the hostel. I visited the new and very impressive Kuala Lumpur International Airport which is some 50-60 minutes drive from the conference venue and discussed with the LOC Chairman plans to meet and arrange transport for participants arriving by air.

Current enrolments for the meeting number 189 and are growing daily. Professor Yamanaka reports that 233 abstracts had been received by 9 July and the table below shows the truly international flavour of the programme that we can expect for the meeting.

Distribution of Papers by Country

Australia 25

Korea 3

Bangladesh 2

Malaysia 13

Canada 1

New Zealand 4

China 7

Sri Lanka 1

England 7

Taiwan 19

France 1

Thailand 5

Germany 1

Ukraine 2

India 23

USA 2

Indonesia 1

Uzbekistan 2

Japan 113

Vietnam 1

The number of contributions to the various microsymbiosia, which have been organised by convenors from the International Organising Committee are detailed below.

MS-01. Diffraction theory (S.L. Chang) 4MS-02.

Synchrotron radiation (K. Ohsumi) 11MS-03. Neutron diffraction (C. Howard) 4MS-04. Electron diffraction (R. Withers) 5

MS-05. Structure refinement by powder diffraction (B. O'Connor) 8

MS-06. Aperiodic structures and incommensurate phases (A. Yamamoto) 8

MS-07. Biocrystallography and protein structure (S.W. Suh)53

MS-08. Organic and organometallic compounds (G. Jameson) 38

MS-09. Inorganic compounds and mineral (T. Yamanaka) 16

MS-10. Materials Chemistry (Y. Ohashi) 11

MS-11. Phase transitions (S.W. Wilkins) 8

MS-12. Charge density (Y. Wang) 5

MS-13. Diffraction under the extreme condition (O. Shimomura) 3

MS-14. Other categories 7

The IUCr 50 Anniversary Symposium to celebrate the anniversary of the International Union of Crystallography will be held in the Main Hall on the morning of Wednesday October 14th. Speakers at this landmark session will be:

Professor Edward N. Baker (Massey University, New Zealand) Chairperson; Professor Tomitake Tsukihara (Osaka University, Japan), Professor C. P. Brock (University of Kentucky, USA), and Professor Aloysio Janner (University of Nijmegen, Netherlands)

Recent progress in various areas of crystallography will be addressed in Plenary Lectures on the mornings of the 13th and 15th. The speakers will be:

Dr H. Kamitsubo (Director of Spring-8, Japan)

Professor Shin-Lin Chang (Department of Physics, Tsing Hua University, Taiwan)

Professor Yuji Ohashi (Department of Chemistry Tokyo Institute of Technology Japan)

Professor Peter M. Colman (Division of Biomolecular Engineering, CSIRO, Australia)

Professor Dongcai Liang (Institute of Biophysics, Academia Sinica, Beijing, China)

The joint efforts of the member of the International Organising Committee, the International Programme Committee and the Local Organising Committee will undoubtedly provide us with an excellent meeting. I look forward to seeing you all in Bangi on 12th October for the start of what should be a most worthwhile AsCA conference.

Jim Simpson)

FUTURE Conferences

ESUM98

European SMART users meeting 1998

A Bruker/AXS Smart users meeting will be held in Bergen, Norway, September 11-13, 1998. Further information can be found on the web page <http://www.kemi.dtu.dk/~nt/Bergen.htm>.

AsCA'98

The third Meeting of the Asian Crystallographic Association is to be held in Bangi in the state of Selangor, Malaysia, from 13-15th October, 1998. The Second Circular has been posted to those who requested it and is available on the AsCA'98 Homepage at: <http://telperion.otago.ac.nz:800/rweavers/ASCA/asca98.htm>. An edited version has been distributed with this *Newsletter* together with the Abstract Submission and the Registration and Accommodation Forms. A call from the Secretary of the SCA for applications for travel awards is on Page 3 of this *Newsletter*.

XVIII IUCR Congress

Glasgow, Scotland, August 4-13, 1999.

The venue for the XVIII IUCR Congress is the Scottish Exhibition and Conferences Centre (SECC) in the centre of Glasgow. The Congress Web page is located at:

[http:// www.chem.gla.ac.uk/iucr99/](http://www.chem.gla.ac.uk/iucr99/)

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The next issue of the Newsletter will be in November. Contributions should be e-mailed to the Editor by October 31

