

NEWSLETTER

Society of Crystallographers in Australia and New Zealand

SCANZ PRESIDENT'S REPORT



Dear SCANZ members,

It has been a big year for crystallography and structural science in Australia with the IUCr 26th Congress in Melbourne. Many thanks to everyone who made it a memorable IUCr: the feedback from around the world was excellent. Special thanks to the conference chair Michael Parker and the organising committee of Brendan Kennedy, Megan Maher, Jack Clegg, David Aragao, Stuart Batten, Melissa Call, Charlie Bond, Helen Maynard-Casely, Emily Parker and Tom Peat.

I had a great time working on the giant diamond model, and found it an interesting way to meet and talk to a different group of scientists than usual. Thanks to Stuart Batten, Helen Maynard-Casely and all of their helpers with the outreach program. I have never seen that number of school children at a conference before.

A final thanks goes to all of those of you who came along and supported the conference. A number of you stepped forward to act as “buddies” for visitors from the Associação Brasileira de Cristalografia, which was welcomed by our South American colleagues. While Jenny Martin completed her term on the IUCr Executive (thanks Jenny!), southern hemisphere representation has increased with the election of Brazilian (Cristy Nonato) and South African (Susan Bourne) as executive members. Opportunities for connections across the Global South have also increased with the African Crystallographic Association being welcomed as a new affiliate to the IUCr.

With the IUCr water now under the bridge, SCANZ can focus on future events. For example, plans are underway for the next Crystallography School, and the next CRYSTAL meeting, so please look out for information about them in the coming months. The SCANZ Council is now in the process of developing a



<http://scanz.iucr.org/>

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strategy for how to use our funds in the best interests of our members and of structural science, so please also expect some communication around this issue in the near future.

Charlie Bond - SCANZ President



IUCR2023 HIGHLIGHTS

Forty-two Maslen scholarships were awarded by SCANZ to PhD students and early-career researchers to attend the IUCR2023 conference in Melbourne. Here are some of their highlights from the conference:



Liam Mckinlay (UNSW)

The first thing that struck me was the sheer scope of the conference itself and that it had managed to encapsulate crystallography from mining ores to protein analysis and everything in between. I had the opportunity to talk with people I didn't even know existed, from joint PhD students from Edinburgh and DESY to people in Australia who are working in the same field as me and offered an exchange of resources between our laboratories. The conference talks and workshops were a highlight to me as well, with the diversity of talks I could always find something that either piqued my interest or made me think critically about my own work. Overall the experience was worth more to me than I could have expected.

Yan Li (UQ)

It is a wonderful experience during my research career. I gained many professional skills from lots of workshops (e.g., CCP4 cryo-EM).

Luke Smithers (UWA)

The highlight of the IUCR meeting for me was definitely the structures of very large assemblies session, in particular the structure of the intact flagellar basal body. I also attended the Phaser workshop, which has been beneficial for my work particularly in docking structures into cryo-EM



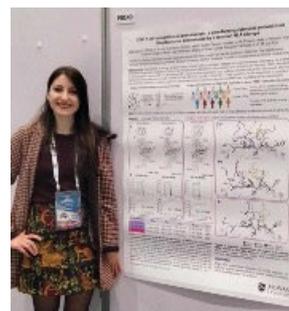
maps. Finally, I enjoyed engaging with people about the bright future of structural biology in a post-AlphaFold world.

Yu Zhang (Monash)

As a student specialising in electron crystallography, I am deeply honoured to receive the SCANZ Maslen Scholarship for IUCr 2023. A stand out moment for me was the presentation of Prof. Jian-Min Zuo. His talk vividly demonstrated the power of 4D-STEM, a key technique in electron crystallography. It left a lasting impression on me. This remarkable congress broadened my perspective on crystallography, providing insights beyond my research area. I extend my heartfelt gratitude to SCANZ for this scholarship, which granted me such a valuable opportunity to participate in IUCr 2023.

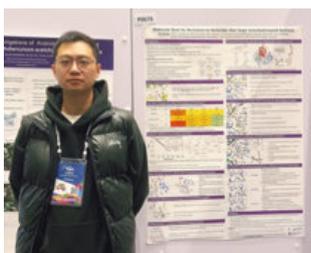
Lisa Ciacchi (Monash)

I enjoyed attending the IUCr2023 conference this year as I gained important insights in how crystallography can be harnessed to answer questions across multiple disciplines, such as in physics, chemistry and biomedical science. It was immensely helpful hearing about advancements made in the software programs used for structural refinement for example, as well as being exposed to talks delivered by world-class researchers who are making profound discoveries and actively working in other disciplines aside from my own area of expertise.



Bikas Aryal (Monash)

International Union of Crystallography conference covered a wide range of talks related to electron diffraction and crystallography. By participating in this conference, I got a chance to understand the fundamentals of electron diffraction and advances in different techniques like 4D-STEM, SEND, MicroED, and Ptychography. Since my research focuses on chemical bonding studies using QCBED, I enjoyed the talk "Measuring vacancy concentrations, chemical bonding and lattice contraction around nanovoids in aluminium by QCBED". Furthermore, this conference provided me with an opportunity to meet world renowned experts such as Jian Min Zuo, Randi Holmestad, and Colin Ophus. I discussed future collaborations with Prof. Zuo. I also met many early career researchers and representatives from different companies. We discussed new research directions and explored industrial collaborations. Last but not least, I am grateful to SCANZ for providing the Maslen award, which greatly aided in covering a portion of the IUCr congress registration fee.



Yan Cheng (UQ)

It was a fantastic experience to attend the IUCr 2023 conference. I obtained some insights into the crystallography related to my studies, especially for enzymes and computational technology in solving structures. Beside this, it was a wonderful chance to talk to the people from other research areas and countries. Thanks also to the sponsors who showed their advanced technology and equipment.

Ben Krinkel (Auckland Uni)

Attending the IUCr was a significant stepping stone in my career of becoming a scientist, as it was my first international conference! I enjoyed the talks on Alpha Fold and how I can use it to assist improving my crystallographic models' geometry. I was also able to network with fellow colleagues and got to meet other crystallographers from all around the world, and the best part was that I won a poster award for my poster!

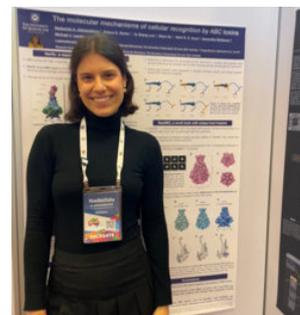
Josh Scadden (Otago)

Over the eight days of the conference, much was achieved from the many talks I attended. Specifically, Tom Terwilliger gave some good ideas about the limitations of AlphaFold that I hadn't considered, Dennis Piehl discussed the modelCIF file format developed for AlphaFold models, and finally Christopher Williams

introduced the MolProbit extension for Phenix to analyse low quality regions. The last of these speakers, Christopher Williams, additionally showed great interest in my poster, asking many questions and could be an avenue for future contact. The two days of my poster also attracted the attention of many other people from around the world, keeping me busy with talks. One other noteworthy source of interest was Gaya Amarasinghe, a researcher at Washington University in St Louis who suggested I could apply for a post-doc position in his lab after I finish my PhD. Overall, I would say the conference was indeed of value, giving me new knowledge, new contacts, and plenty of free stuff from the sponsors.

Nadezhda Aleksandrova (UQ)

IUCr 2023 was an amazing opportunity to network with the best crystallography researchers from all around the world! The talks that stood out to me most were in the session on Intracellular crystallography, and in particular the talk from Prof Lars Redecke on new approaches in intracellular protein crystallography in insect cells- an exciting novel technique for protein structure determination. In addition to the scientific programme, I thoroughly enjoyed taking part in the informal networking events- building the Big Crystal, the Rigaku Fun Run, and the Congress celebration at the Melbourne Museum.

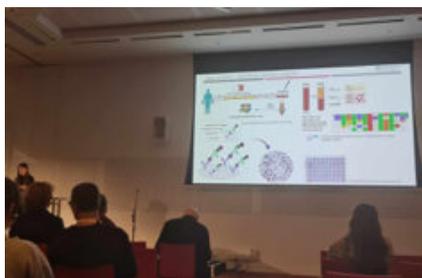


James Brookes (UWA)

The IUCr in Melbourne 2023 was an immense success. Through the many interesting and wide ranging microsymbiosia, and fruitful discussions with fellow crystallographers from diverse backgrounds, I was able to gather a lot of new information and ideas. The knowledge that I gained through attending the congress will greatly improve my PhD project and created exciting future career endeavours. I was lucky enough to present a poster of work for the first time, which gave me invaluable experience in presenting scientific results, and also allowed for my work to be viewed by people from outside of my research group, their fresh eyes bringing new perspectives from a diverse range of crystallographic disciplines. The positive impact of being given the opportunity to meet with researchers from around the world will be long lasting, with connections made hopefully leading to future collaborations and exciting science. SCANZ and the Maslen scholarship were instrumental in allowing me to attend this congress and gain this invaluable knowledge. I would like to thank SCANZ and IUCr for their efforts in organising and running this congress, everything ran incredibly smooth with no problems whatsoever. The immense amount of work that went into this event was noticed and greatly appreciated.

Laura Ciacchi (Monash)

It was a privilege to attend and present a talk at the IUCr2023 conference. I have gained more insight into the complexity of crystallography and the many exciting new technologies to assist us with current tools for structural modelling and refinement. I enjoyed learning about different fields within crystallography ranging across its use in dating artworks, techniques to improve crystal growth and validation of structures and fragment screening drug candidates. I enjoyed learning of the timelines expected for new developments in computing technologies and validation tools that will assist crystallographers in the future. This was also a great opportunity to network with leaders in the field as well as meeting fellow ECRs.

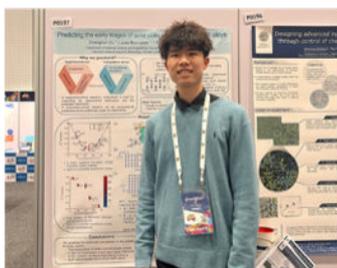


Nicholas Stapleton (UWA)

Overall, the IUCr2023 Melbourne conference was a great success, informative for my research, and provided opportunities to learn and connect with experts in the field. The workshops I attended before the official conference opening were good learning resources for planning experiments at national facilities (namely, Synchrotron light sources) and use of analysis software for single crystal data. There were several microsymbiosia throughout the conference which covered material relevant to my research. In particular,

the powder diffraction session outlined good techniques for experiments and post-experiment analyses, which both illuminated new approaches and confirmed methods I was already employing. I also contributed towards building small segments for the big diamond model organised for the Bragg Your Pattern project, which broke the world record for largest diamond structure made from plastic model kits. On the final day of the conference (29th August), I delivered a 15-minute oral presentation of my research at the Crystallography in Space Research microsymposium. I presented results from my computational study of Titan-relevant molecular cryominerals, briefly outlined my experimental work at UWA and Australia's national facilities, and acknowledged financial assistance given by SCANZ. The microsymposium had a high audience turn out (upwards of 40), and I was able to chat briefly with the session chair and a few of the other presenters (based in the US, Japan and Australia).

Multiple poster sessions ran throughout the conference, providing good opportunities to communicate with other researchers. On the last two days of the conference (28-29th of August), a handful of posters relevant to crystallography in space research were displayed, where I met a PhD student from the University of Otago whose research also focuses on Titan-relevant molecular co-crystals. We were able to have several fruitful discussions about useful techniques and approaches in the field, as well as relay a few recent developments in Titan cryomineral research from our own experiences and experiments. It may be possible for us to collaborate in the future due to similarly aligned interests and research goals.



Shenghan Su (Monash)

During my participation in IUCr2023, I had the opportunity to engage in fruitful discussions and unexpected collaborations with researchers. Presenting my poster attracted many questions, with one exchange of contact information for future collaborations. The most useful information for me is the use of deep learning algorithms for crystal structure screening, potentially saving me significant research time.

Helen McGuinness (UQ)

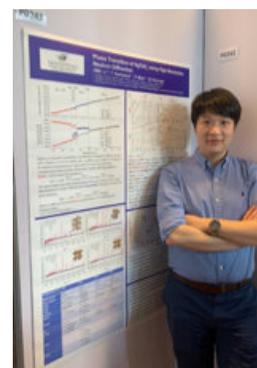
My first IUCr congress was a fantastic experience – Tom Terwilliger's talk on how AlphaFold changes "everything, and nothing", was particularly inspiring, forecasting a bright future for structural biology with the integration of experimental data and structure prediction. With attendees from all over the world, I was struck by the feeling of community at this conference, from enthusiastic discussions in front of posters, to meeting people while building the #braggyourpattern big diamond structure! Thank you to SCANZ for enabling my attendance at IUCr 2023 by supporting me with a Maslen scholarship, and I look forward to attending IUCr 2026 in Calgary, Canada.

JW Ben Li

Favourite talk: Magnetic PDF by Dr Benjamin Frandsen

Networking opportunities: had great chat about the uses for neutron powder diffraction, able to let potential users know that the high resolution powder diffractometer at CSNS should be able to accept users in 2024. Discussed with beamline scientists from Australian Synchrotron Powder Diffraction beamline about potential experiments.

Useful insights: Different uses of PDF on magnetic systems, the use of crystallography other than materials research such as geology, study of artefacts, astronomy, etc.



Isabelle Jones (UWA)

The opportunity awarded to me to attend the IUCr2023 conference was immensely rich and rewarding. Not only was it amazing to see the breadth and depth of research covering all corners of crystallography (and anything covering crystallography in space is an absolute bonus), but the opportunity to meet and network with vendors and researchers alike was unparalleled. A particular highlight was networking with the vendors, discussing potential collaborations and future careers, and discussing the upcoming features in their systems that I may be able to put to use.

Outside of my favourite talk discussing the collection and classification of meteors in Australia (outside the scope of my work, but who doesn't like space rocks?), I especially enjoyed the keynote presentation by Daniel Bowron discussing the examination and analysis of disordered systems (including gas uptake) by neutron diffraction, which was highly relevant to my research and generated quite a few ideas.

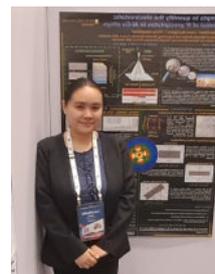
After my presentation, I had the welcome opportunity to discuss the results, and improvements to my loading methods, with other researchers that generated more ideas and potential for collaboration for the research going forward.

This opportunity and experience would not have been possible without the support of SCANZ and the Maslen scholarship, for which I am so grateful.

Loreibelle N. Abian (Monash)



The best talk that I attended was Prof. Joanne Etheridge on the topic of Finding the atoms that matter in functional materials for it tackled one of the fundamental issues in crystallography and microscopy. Moreover, I presented a poster about my research and was awarded a poster prize by ACS Publications Journal-Crystal Growth & Design. I would like to extend my gratitude to SCANZ for the sponsorship to attend IUCR2023.



Andrew Marshall (UWA)

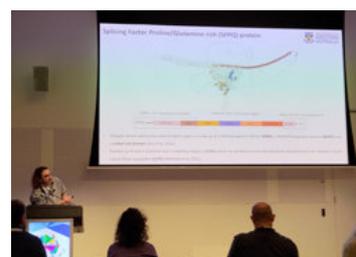
Of the many amazing talks, my favourite would have to have been Prof. Xiaodong Zhang from Imperial College London walking us through beautiful structures of RNA polymerase showing how double-stranded DNA is melted to allow transcription.

I really enjoyed the interactive CCP4 and CCP-EM pre-conference workshops – having a free webserver for all steps of protein structure solution and model building is amazing (I solved my first structure via the browser on my phone!)

Even more than the outstanding science, my highlight was meeting and connecting with other protein scientists from Australia's east coast, Japan, the UK and the US, most of whom I hadn't met before. The poster sessions gave me opportunities to learn about applying NMR to studying disordered proteins, high-pressure crystallography to capture different conformations of protein flexible regions, and secure a possible collaboration working on plastic-degrading enzymes.

Heidar Konig (UWA)

I recently attended IUCr 2023 with the help of the Maslen Award and gave a talk on important multipurpose proteins that are involved in mammalian gene regulation. This was one of my first bigger experiences with science communication outside of Western Australia and I'd love to do something similar again. Amongst many, my favourite talks were about the crab claw-like structure of RNA polymerase and how cryo-EM was used to capture the complex in several complicated states. I also really enjoyed the talk about how meaningful information can sometimes be extracted from AlphaFold regions with poor pLDDT scores.

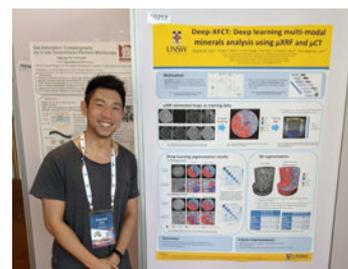


Frederick Marilton (UTS)

At IUCr2023 I was fortunate to share my work with an engaged audience regarding disorder of functional materials. IUCr2023 created the opportunity to host a total scattering workshop in Sydney where we had great international speakers and a significant number of attendees. This provided more opportunities for local researchers to learn and network with experts in the field.

Patrick Tung (UNSW)

At the recent IUCr conference in Melbourne, the standout talk by Arkadiy Simonov presented groundbreaking research into the latest advancements in disordered structures, and delved into standardising the field in order to be able to establish a conventional approach for analysis. Beyond the sessions and the networking opportunities, the Night at the Museum conference event was especially unique and memorable.



ELECTRON CRYSTALLOGRAPHY SCHOOL

Monash University

By Laure Bourgeois and Aaron Gosling

On 19-21 August 2023, the Monash Centre for Electron Microscopy (MCEM) hosted the Electron Crystallography School 2023 (ECS2023), as a satellite event to the 26th International Union of Crystallography (IUCr) Congress and as a Microscopy Australia Masterclass.

The ECS2023 focused on two broad topics that have seen considerable development in the last decade or so: 4D-scanning transmission electron microscopy (4D-STEM) and 3D/micro-electron diffraction (3D-ED). These developments have led to major advances in the characterisation of the atomic-scale structure of solid matter, from energy materials and green chemicals to glasses, proteins and pharmaceutical compounds.

The School was aimed at postgraduate students, early career researchers and new comers to the field. It offered a series of lectures on the fundamental theory underpinning 4D-STEM and 3D-ED, together with historical background, software demonstrations and hands-on tutorials. The intensive program also included a live demonstration on MCEM's latest transmission electron microscope acquisition, the Thermo Fisher Scientific Spectra-j. A session was dedicated to presentations from industry scientists. There was also a lively poster session and a tour of MCEM facilities.

The School was very fortunate to have twenty distinguished scientists from both overseas and Australia as its speakers. Amongst them were Ute Kolb (Johannes Gutenberg Universität Mainz) and Jian-Min Zuo (University of Illinois), past and present recipients of the Gjønnnes Medal in Electron Crystallography, the highest distinction in the field.



The ECS2023 included presentations from many distinguished international scientists, here Prof. Lukáš Palatinus from the Czech Academy of Sciences (photo courtesy of Steve Morton).



Group photo of the Electron Crystallography School 2023 on a sunny afternoon at Monash University (photo courtesy of Steve Morton).

Over 70 delegates from 13 countries and 4 continents attended the School, with students and researchers from countries as far away as Brazil, Belgium and China. This included a significant cohort from the X-ray crystallography community. Feedback from attendees was very positive, with appreciation shown not only for the quality of the program, but also for the opportunity to meet with the broad crystallography community.

The two co-chairs of the organising committee, Hongyi Xu (Stockholm University) and Laure Bourgeois (Monash University) are grateful for the generous support from the following sponsors: Microscopy Australia, the IUCr, the Society of Crystallographers in Australia and New Zealand (SCANZ), Rigaku, JEOL, Thermo Fisher Scientific, Dectris, ReadCrystal, Gatan Ametek and NanoMEGAS.

CRYSTAL-A-CON

The first pop-up Crystallographic Science Festival

By Helen Maynard-Casely on behalf of the team:
Rosie Young, Emily Furlong, Bryce Mullens, Stuart Batten

If you ventured to the back of the exhibition hall during the recent IUCr 2023 congress, you would have found the latest adventure from the [Bragg Your Pattern](#) team – a pop up science festival Crystal-A-Con.



The world-record Diamond attempt proved a popular networking spot for delegates of IUCr2023, as well as a big draw as an interactive activity during Crystal-A-Con. Photo Credit Thomas Proffen

constructed into a giant diamond model over only 4 days. Not only did this provide a fantastic networking opportunity for delegates, but the eventual goal is that the diamond structure will be pulled apart into kits for schools all over Australia and New Zealand as an on-going education resource.

Look out for more about the project in a write up for the IUCr December newsletter and expect more going forward from the Bragg Your Pattern team.

Over 400 members of the public were welcomed during three half-day sessions, taking part in seven interactive activities and enjoying crystallographic installations. Visitors had the opportunity to make their own model virus, construct a sweeter version of the salt crystal structure and explore patterns of the world. Taking advantage of the world's crystallographers who had descended onto Melbourne, a series of 'meet the crystallographer' short talks were held, hearing from scientists from Switzerland to Uruguay.

But perhaps the most memorable activity would be the attempt to break the world-record for the largest crystal structure model. Crystallising the expertise of the conference, over 62,000 carbon atoms were



Bragg Your Pattern competition winners' art was displayed on our giant buckyball.



A big thanks goes to all who helped make Crystal-A-Con a reality, including many staff at Australian Synchrotron. From giant structures to sweet crystals, Crystal-A-Con had it all.

SCANZ president Charlie Bond supervises the last carbon atom being placed by Stuart Batten. Photo Credit Jun Ashima



The Bragg Your Pattern team; Emily Furlong, Stuart Batten, Bryce Mullens, Helen Maynard-Casely and Rosie Young

MAUREEN MACKAY AWARDS



Photo: Cabrini Foundation

SCANZ recognises that that caring responsibilities can severely interrupt, delay or otherwise constrain academic careers and that conference attendance is critical to career development, forging new collaborations, raising researcher visibility in the community and generally enriches scientific research.

This new award (established in 2023) is provided to Society members who need financial assistance to offset the primary carer responsibilities associated with national or international conference attendance. The award is in recognition of the significant contributions of Maureen Mackay to the field of X-ray crystallography in Australia.

Maureen F Mackay started her career path in small molecule crystallography quite by chance. As a chemistry graduate in the early 1950s, she travelled to Oxford with her then husband Donald to begin his D.Phil, where they stayed with Dorothy Crowfoot Hodgkin, receiving accommodation in exchange for childcare and other help. Dorothy encouraged Maureen to work part time in her laboratory on the crystal structure of morphine, which ultimately led to her first publication. She also helped with the crystal structure of vitamin B₁₂, which contributed to Hodgkin winning the Chemistry Nobel Prize in 1964 (the third woman to do so). Maureen completed her PhD under Sandy Mathieson and was subsequently the first woman to be appointed to the Physical Chemistry staff at La Trobe University. She remained at La Trobe where she carried out research into molecules of biological interest. Maureen was the first female Australian to chair a session at a Crystal Meeting (Crystal 19 at Ballarat in 1995). She was also the first woman to occupy a named position (Treasurer, 1982 - 1987, Council member 1987 – 1993) in the SCA (which preceded SCANZ).

This award will support the cost of arranging alternative care while the applicant is attending a conference. For example, applicants may require additional care at home to allow them to travel or may use the award to provide care at a conference venue, including providing funds for an alternate carer to travel with the applicant, and/or the cost of the dependent's travel if there is a need for them to travel with the applicant.

Please keep an eye out for emails from the SCANZ Secretary with details regarding the application process and due dates. Please also spread the word around your institution to people who might benefit from this award.

SANDY MATHIESON MEDAL

The Sandy Mathieson Medal recognises distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging by a mid-career researcher. The award is open to members of SCANZ (for at least the previous five continuous years) with up to 15 years of post-PhD experience (taking into account any career interruptions).

Applications for the 2023 Sandy Mathieson Medal are now open, and will close on 31st October. All documentation, including referee reports, must be emailed to the SCANZ Secretary (secretary@scanz.org) prior to midnight on the closing date.

LIFE MEMBERSHIP NOMINATIONS

We are looking for nominations for Life Members. If you know of anyone who you think fits the criteria below and should be nominated, send an email to the SCANZ Secretary (secretary@scanz.org) to let us know.

Honorary Life Membership of the Society may be granted to a person pre-eminent in Crystallography and/or one who has rendered conspicuous service to the Society. A nomination for Honorary Life Membership shall be sponsored by three members of the Society, and shall be accompanied by a supporting citation. Election of the candidate shall be by the full Council and shall be confirmed by a majority of at least two-thirds of those voting at a duly announced Business Meeting.

NEW MEMBERS WELCOME!!!

SCANZ welcomes new members, particularly from New Zealand. Benefits of membership include:

*Global representation through ASCa, IUCr and STA
Prestigious Awards
Discounted conference fees
Exceptionally generous student travel support
Information and job vacancy sharing
Membership from as little as \$10 per year for students*

Membership applications can be made through the SCANZ website, contact your friendly SCANZ committee members if you require a sponsor for your application.

<https://scanz.iucr.org/>

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