

Journals Management Board meeting

Chester, UK, 16-17 March 2023

Chair: Andrew Allen

Attendees: Andrew Allen (IUCr Editor-in-chief), Simon Billinge (*Acta A*), Sandy Blake (*Acta B*), Hanna Dabkowska (IUCr President), Elspeth Garman (*Acta D*), Janos Hajdu (*JAC*), Bill Harrison (*IUCrData*), Loes Kroon-Batenburg (*IUCrData*), Kristina Kvashnina (*JSR*), Sean Parkin (*Acta E*), Thomas Proffen (Commissioning Editor), Mark van Raaij (*Acta F*), Paul Raithby (*Acta C*), Randy Read (*Acta D*)

Chester staff: Nicola Ashcroft, Amanda Berry, Sean Conway, Simon Glynn, Gillian Holmes, Mike Hoyland, Louise Jones, Ed Morgan, Andrea Sharpe, Lisa Stephenson, Alex Stanley, Peter Strickland, Tony Weight, Simon Westrip, Michele Zema

1. INTRODUCTION

The Editor-in-chief welcomed everyone to the meeting. The journals were generally doing well but it was important to think strategically to address the changes and challenges they are facing. In general, authors report very positive experiences publishing with the IUCr.

Much has happened since the last in-person meeting. Commissioning Editors have been appointed, as have many Co-editors, trying to improve the diversity of the editorial boards in terms of gender, geographical spread and subject area. Our team of over 200 volunteers really does make the journals work. Many special issues have been published and three new sections launched – Electron Crystallography in *IUCrJ*, Crystal Growth in *Acta B* and Raw Data Letters in *IUCrData*. In addition, new initiatives are strengthening the connection between *Acta E* and IUCr outreach activities.

It is important to keep the journals relevant over the coming years by launching new sections. One major challenge is the fall in the number of submissions, another is that all articles are likely to be open access within a few years. Diligent review with everyone treated fairly is core to the journals and this must be maintained whilst exploring how to improve the way we work. Getting the Co-editors to feel a sense of ownership and feel empowered to make suggestions, and to be part of the organic growth of the journals will be helped by regular editorial board meetings. We need to be prepared to adapt to changes in the way that crystallography is perceived by the wider scientific community and be prepared to be innovative in attracting new authors. Finally, post pandemic, we need to explore new ways of promoting the journals.

Alex Stanley, the IUCr CEO, then described plans for the rebranding of the IUCr. The essence of the IUCr encompasses its sense of community, its contribution to world-leading research and its high-calibre publishing. A welcoming and inclusive organisation, it is well established and recognised. Headwinds include publishing model changes, reduced submissions, increasing costs and the competitive publishing landscape. The help of the editors is needed to brainstorm on areas from social media to special issues, all with the focus of increasing high-quality submissions.

2. MAIN ISSUES TO ADDRESS AT THIS MEETING

The key issue is increasing the number of submissions while maintaining the quality of the journals. Various ideas for achieving this were discussed throughout the meeting, with breakout sessions where the chemistry (*Acta B, C and E*, and *IUCrData*), biology (*Acta D and F*), and materials, methods and instrumentation (*Acta A, JAC, JSR and IUCrJ*) editors, with input from the Executive Managing Editor, the Editor-in-chief, the IUCr President and the IUCr Executive Outreach Officer, considered strategies and ultimately came up with an action plan for each of the journals (given at the end of these notes).

3. JOURNALS DEVELOPMENT

3.1. Brief reports by Main Editors, including matters arising from editorial board meetings

Acta A

Simon Billinge reported that the journal is essentially healthy. The impact factor is above 2, but he would like it to be higher. The virtual editorial board meeting had been successful. Previous efforts to increase submissions and widen the scope had been unsuccessful because of a mismatch between aspirations and the ability to deliver. Special issues and Lead Articles had been commissioned but failed to appear. Attempts had been made to widen the scope beyond crystals, but changes to the rubric and new Co-editor appointments had not brought in submissions. The journal plans to commission short, templated ‘best practice’ articles from top researchers in subject areas it wants to encourage. Pre-screening has been discussed to address the issue of adding relevance to papers, as efforts to get authors to do this at a later stage have not been successful. Another challenge is long review times.

Acta B

Sandy Blake reported that the journal is attracting submissions but the number of papers in the system is much reduced. There had been concern about how the war in Ukraine would affect submissions. In 2021, the top two countries publishing in the journal were Poland (18%) and Russia (15%). In 2022, Russia was still in second place with 11% of submissions while Poland had dropped to third place (9%). Commissioning high-impact articles has not been successful but special issues have done well, with articles having good impact, and more are planned. The high impact factor of the MDPI journal *Crystals* was noted. This journal publishes a lot of materials science papers, an area that should be covered more in *Acta B*.

Acta C

Acta C is a key journal in terms of the large subscription revenue it generates but submissions have continued to fall. Paul Raithby reported that they are still trying to broaden the audience for the journal. The first editorial board meeting had been very positive, with Co-editors willing to work to improve the journal. One special issue had been published recently and more were in the pipeline.

Andrew Allen noted that the future role of *Acta C* needs to be defined. Problematic fields such as how to use AI to solve structures could form the basis of a new section for *Acta C*, provided suitable Co-editors are identified and recruited.

Acta D

Randy Read reported that while the impact factor had remained above 5, it was based on only a small number of papers. Submissions were holding up. Although cryo-EM has increasing impact, the journal had not been successful in capturing papers, although publishing papers from CCP-EM meetings does raise the profile of *Acta D* in this area. AlphaFold has changed the landscape of protein crystallography and the journal needs to make sure that it publishes the whole picture – not just how the structure was solved, but the underlying biology as well. It is now mandatory to submit structural data.

Acta E

Sean Parkin reported that the biggest change will be the journal regaining an impact factor, which could lead to a large rise in submissions, particularly from China. New Co-editor appointments are being worked on and a good candidate from China has been sounded out informally and is willing to serve. A Jerry Jansinski special issue was published recently and a teaching one is ongoing. The teaching papers have been well received and cited. The journal is looking to appoint a Co-editor for powder diffraction to increase submissions from this community and a special issue will be

considered. Jim Kaduk, who has published extensively in *Acta E*, was suggested as a Guest Editor. Other special issues on perovskites (Mike Glazer) and nanotechnology were suggested at the meeting.

Acta F

Mark van Raaij reported that the number of submissions to *Acta F* was going down and that the journal was rejecting more papers than five years ago. It is important that the journal distinguishes itself from *Acta D*. Andrew Allen noted the need to define the future role of *Acta F*. There are plans to focus on sample preparation for all the different structural biology methods, combined with attracting more early career researchers. Short, narrow in scope, methods papers and topical reviews could be published, along with papers describing experimental facilities. *Acta F* could also have a role documenting unpublished PDB entries.

JAC

Janos Hajdu reported the journal was doing well, but that there had been a drop in submissions of about 14% since 2017. The rejection rate had gone down but the quality had improved. The proportion of open-access papers had increased tremendously. At around six months, the average publication time is too long. A special collection of articles on AI is being assembled. Problems in working on the special issue were noted.

JSR

Kristina Kvashnina reported that *JSR* submissions are down by about 10% (this is less than predicted following the transfer to open access) but that the quality of papers has increased. *JSR* became fully open access in January 2022. The proportion of submissions from China, France and the USA has increased, but there have been decreases in the proportion of papers from Germany, Japan and Sweden. Experience with special issues has been very positive. The latest on actinides contained around 20 papers and all those invited to submit papers did so. Three special issues are planned for 2023. The virtual meeting of the editorial board went well and new Co-editors are being mentored. The Main Editors are working to raise the impact factor and increase submissions while reducing the publication time.

IUCrJ

Andrew Allen reported that submissions to *IUCrJ* are down. A new section on electron crystallography has been launched. Forthcoming Main Editor retirements and new appointments may result in a slight change of direction. No special issues have been published so far, but ideas for small, high-impact, cross-cutting special issues are being explored.

IUCrData

Bill Harrison described the exponential decline of submissions to the Data Reports section. It was necessary to decide how to move forward, considering the synergy with *Acta E*. Andrew Allen noted the need to cater for emerging FAIR data requirements. Loes Kroon-Batenburg described the role of Raw Data Letters in the light of open science-driven research. A lot of effort had been put into developing tools for preparing and checking imgCIFs. More submissions are needed to complete that work, which represents a big step forward in data quality and validation. Three Raw Data Letters have been published so far. Andrew Allen said there had been a push for raw data availability for many years and it was clear that Raw Data Letters could serve as a template for moving forward with data curation for the journals. Many funding agencies are moving forward to mandating that data and metadata are findable, and *IUCrData* can work on these issues.

General, including matters brought up in breakout sessions

The distinction between *Acta B*, *C* and *E* was discussed. It was felt that there is a continuum between *Acta C* and *E*, but that *Acta E* is also carving out a distinct identity in developing the teaching aspect and its role allied to the IUCr's outreach activities. *Acta B* is more concerned with properties and function, and *Acta C* with synthesis and structure. *Acta C* really needs to find its own niche, possibly in quantum crystallography as the board has expertise in this area. There could also be possibilities for a partnership with *IUCrData*. Efforts to attract the synthetic chemistry community have not been successful, so it will be necessary to explore other options, starting with the computational side of crystallography (AI, CIFs that have not come from diffraction experiments etc.) with appropriate expertise recruited to the *Acta C* board.

The scopes of *Acta D* and *F* were also considered. The subject areas covered are essentially the same. The journals will be referred to more by their subtitles. Sample preparation is an area that may become more important for *Acta F*.

All journals need to review and update their scopes before Congress, making sure that important areas, such as powder diffraction, are covered. It would be good to note that the scopes are being revised in the report to the General Assembly. It was also noted that the new journal scopes could be publicised by adding a sentence or two to standard emails.

It would be useful if the journals were able to contact attendees of outreach events. Applicants to OpenLabs could be asked to agree to the journals contacting them. Also, a box to tick on submission if it is an author's first paper could ensure new authors get extra help, including making sure that their paper is publicised on social media.

Early career researchers can find it difficult to decide where to submit. A web page with the scopes of all journals could help. This could include a tool to help authors decide based on the abstract and/or keywords.

It was felt that pre-screening could be an important element in speeding up publication for some journals. It was also noted that it was important that Co-editors are aware of the transfer process between journals.

The popularity of getting your paper on the cover was discussed, along with the possibility of involving the author's institution in producing a really good image.

Finally, it was thought that Co-editors should be encouraged to be ambassadors for the journals when attending meetings, and publicity materials can be sent directly (and internationally) to conference desks for pickup and dissemination by attending Co-editors upon their request to the Chester office.

4. REFEREES AND THE REVIEW PROCESS

Peter Strickland gave a demonstration of the Prophy system for generating suggestions for reviewers. The IUCr has this on a two month trial. It is used by the European Research Council and seems to be well respected by them. PDFs of articles are uploaded and then analysed. Suggestions for similar articles or referees are generated from its database of around 140 million articles. Information such as affiliations, email address, h index, citations, journals published in, and papers published are given for prospective referees. It also tracks where people have worked over the years. The user can fine-tune the filters, for example to exclude date ranges or select a younger academic age (as less senior people may actually have the time to do a review). It identifies topics in the paper and these can be boosted or excluded as required. We would need to consider how this integrates with our systems, but it has the potential to be a big help in finding referees who will actually be interested in reading and reviewing a given paper.

Papers written by some of the editors present at the JMB had been entered into the system. They will be sent a spreadsheet of suggested reviewers generated by Prophy and will be asked to review the recommendations and give feedback.

Peter reported that the new review system is in place. There had been useful feedback from Co-editors. The Co-editor handbook has been updated but more in-context help needs to be added to the review pages.

Review and revision times had been looked at. Charts have been generated that showed that some papers had long review

times, and also showing how long each stage of the process took. Articles can get stuck at any stage of the review process and we need to look at which stages to target. Automatic reminders will be generated, and an interface provided to show articles that are stuck in the system. It was felt that alerts should not just go to the Co-editor, as Main Editors might need to get involved and send friendly reminders, and offer help if needed, if the Co-editor is not responding. In the current system, it is very difficult to work out where a specific delay is. We need to make sure that any solution is not a burden to Co-editors and does not bombard them with too many emails.

It is necessary to alert reviewers that there is supporting information that needs to be reviewed with the rest of the paper. Ideally, the review document should be generated to include the supporting information. It was agreed that a question about supporting information should be drafted that could be added to the usual questions for referees. Improved guidelines for reviewers will be worked on – it will be important that they are brief and to the point. The guidelines will be sent out to the Main Editors for feedback. Training for reviewers was discussed, including producing the new guidelines and the possibility of a workshop at Congress.

There was discussion on how to handle Co-editors who are rude to authors. It is good to discuss situations such as these, which need sensitive handling, with Main/Section Editors, the Editor-in-chief or the Chester office. They should be handled on a case-by-case basis.

The problem of referee comments on revised articles not being transferred to the system was raised. An update to the system should be able to handle this matter.

5. SPECIAL ISSUES AND COMMISSIONING

Special issues

Andrew Allen said that special issues work best where there are two Guest Editors, one of whom is already on the Editorial Board. Guest Co-editors can be invited, depending on the number of papers anticipated, with individuals handling a maximum of 4 or 5 papers. Submissions should go through the normal review process – authors of other papers in the special issue could be used as referees. Accepted papers are posted online and published in regular issues with full citation information, when ready, then collected into a virtual special issue, along with a foreword that describes and cites each of the papers.

Joint special issues across journals

Cross-journal special issues can be a way of getting a wider range of papers. These could arise out of new sections in the journals.

A collection of papers associated with AfCA will be published across the journals, but mainly in *Acta C* and *E*, and *IUCrData*. It will also include feature articles on education and development initiatives with the focus on science. It is hoped that a few articles will be online by Congress.

Special issues in other journals could also follow on from small, high-impact, cross-cutting special issues being explored for *IUCrJ*, for example on structure prediction (edited by Richard Catlow). It is hoped that the next structure-prediction blind test paper will be published in *Acta B*, and this could be used as a springboard for special issues across the chemical journals.

It needs to be clear who is taking responsibility for cross-journal initiatives, and tasks need to be finite.

Commissioning

It was noted that for some journals, commissioning individual articles is more tractable, while for others attracting papers

for special issues is more successful. It was also thought that it might be easier to commission short papers that are not such a big project for authors. This was certainly the case for Scientific Commentaries, where a good reviewer can generally be commissioned to write a quick commentary.

We should be more systematic in identifying which meetings Co-editors are attending and in asking them to suggest possible authors and special issues. Empowering Co-editors to be more proactive can be achieved by holding regular board meetings.

Commissioning Editors

The Commissioning Editors were appointed three years ago. Communication seems to have been an issue, and from discussions at the meeting, it was clear that their role is not well understood, even by the Commissioning Editors themselves. Andrew Allen will work to clarify this. He felt they could make a major contribution in the long term. About 20-25 papers have been commissioned to date, including a high-pressure special issue in *Acta B* and a room-temperature special issue in *Acta D/Acta F/IUCrJ*.

International Tables

Nicola Ashcroft said that at present there were ten *International Tables* volumes, with the latest, Volume I, going online article by article. Most volumes are active with new revisions online or in prospect. They contain authoritative reference articles and review-style articles. Nine volumes are in print and the online version is hosted by the IUCr. Wiley also hosts PDFs, with links back to the IUCr website for html.

There are currently a number of problems. It is becoming increasingly difficult to commission articles as they are not included in citation metrics. It also takes considerable time to collect enough articles for a volume, and articles may be out of date by the time the volume is published. In addition, print sales are falling with unit printing costs rising. Some institutions are now mandating open access for articles in books.

Nicola described a proposal to publish all new *International Tables* articles in the most relevant journals first. There would be new journals sections called, for example, *International Tables* reviews or IUCr reviews. The *International Tables* editors could work with the journals to propose authors and topics for articles (including in areas they think the journals should move into), to identify the most appropriate journal and to assist with referees. After publication, a link to the article would be added on the *International Tables* website. Subscribers would be able to access all new articles, whether open access or not. *International Tables* online would become a collection of older material plus a virtual collection of journal articles, not necessarily sorted by journal.

Advantages of this proposal include recognition for the authors, citations to the articles and faster publication. It would also be easier to offer open access. The articles are likely to be highly cited, which would be good for journal impact factors. However, *International Tables* subscription revenues would be likely to decrease, although this should be balanced by an increase in open-access revenue. Ultimately, the same funding model as for the journals would apply. The aim would be to publish around 50 articles per year.

Currently, articles are commissioned for a specific volume and this means that there may be many reviews in a specific subject area, which could swamp a journal. In the longer term, articles would be commissioned across subject areas so this would be less likely to be a problem.

Issues such as how the *International Tables* editors would be involved in the review of a paper and how to handle cross-referencing were discussed.

Attendees of the meeting were enthusiastic about the proposal, feeling it offered a much more flexible approach that would benefit the journals.

6. OPEN ACCESS AND OTHER PUBLISHING DEVELOPMENTS

Open access

Peter Strickland described the IUCr's experience with open access since 2003, including JISC funding in 2004-2007, *Acta E* flipping in 2008, the launches of *IUCrJ* in 2014 and *IUCrData* in 2016, the first Wiley 'read and publish' agreements in 2018, modifications to licensing to conform to Plan S in 2019, and flipping *JSR* in 2022. More open-access revenue is now obtained from Wiley than direct open access, the proportion of open-access papers in our hybrid journals having risen to 45% from 32% in 2020.

Flipping *JSR* to open access has gone well so far, with submissions holding up, although the number of waivers is higher than expected.

Over the next few years, we expect to continue working with a publication partner on our hybrid journals and to self-publish some open-access journals, for which we will seek to develop and market 'pure publish' deals. We will continue to monitor what other learned society journals are doing, and explore other models. Full open-access publishing is anticipated within 5-10 years.

7. OPEN DATA AND DATA REQUIREMENTS

The IUCr has adopted a data-sharing policy that requires the crystallographic data supporting the results in an article to be peer reviewed and archived either with the IUCr or in an appropriate public repository. The *Notes for authors* of journals covering macromolecular structure determinations have been modified to strengthen requirements for the reviewers to be able to access the underlying data. The *Notes for authors* of other journals will be updated over the next year.

Over 100000 data sets accompany our journal articles, and we are exploring what might be done with these, for example how they might be made more accessible to the community. There may be services that can be charged for.

8. OTHER EDITORIAL MATTERS

AI tools

It was agreed that we should follow other publishers in not allowing an AI tool to be a named author of an article. Any use of an AI tool in preparing an article should at least be noted in the acknowledgements. It was felt that if software such as ChatGPT is used as a tool, then it should be reported as such, for example the methods or acknowledgement section could state 'the first draft of parts of the Introduction was written with the assistance of ChatGPT'.

Titles in references

The Editors present found the inclusion of titles of references to be useful, and thought that this would also be beneficial for referees. Options will be explored, including using titles given by authors, adding titles, mouse-over in the online version, etc.

General

The issue of multiple covers was discussed - it is a pity to only have one cover if there is more than one good candidate.

It was also stated that papers are tending to get longer. It was not felt appropriate to set limits on their size, but it could be appropriate to move material into the supporting information. Basic supporting information should be referred to in the text, but it is not necessary to cite every section in the supporting information. A useful feature that could be added to the results page when searching for papers on a particular topic in IUCr journals would be to include tick boxes that researchers could use to select which papers they were interested in, allowing them to then download the references in a format of their choice for adding to a bibliography.

9. TOOLS AND TECHNICAL DEVELOPMENTS

Various projects that are being worked on are described elsewhere in these notes.

10. PROMOTIONS/MARKETING/ARTICLE HIGHLIGHTING

Andrea Sharpe described changes to the marketing department, including the appointment of Ed Morgan as an apprentice. As part of the rebranding exercise, new social media templates have been produced, along with thank-you e-cards for referees. There is a greater emphasis on reaching out to other areas of science and driving an increase in submissions, and also on digital marketing. We aim to take advantage of services offered by Wiley. Possibilities include contacting potential authors eligible for free open access, and sending certificates to authors of top cited and most downloaded articles. The *IUCr Newsletter* continues to include reports on new developments such as new journal sections, and to highlight special issues and commentaries. Social media coverage has increased and new methods of engagement are being assessed. IUCr poster prizes continue to be well received, and it is good if they can be presented by someone associated with the IUCr. This can be a Co-editor of the relevant journal who is attending the conference. Promotional material for meetings continues to be produced and plans are underway for the Melbourne Congress, such as an early-career researcher video competition, best paper/cover awards and merchandise branded with the IUCr75 logo.

Andrew Allen suggested that each journal should have a slide advertising the journal, or a particular aspect of it, that could be shown at the end of talks. Editors attending meetings where we have a stand should be encouraged to visit the stand and talk to attendees.

It was felt that structural science should be emphasised in marketing, rather than crystallography.

It was thought that not having a branded store was a missed opportunity.

An exercise is being undertaken to refresh the vision and values of the IUCr, and editors are encouraged to take part in the accompanying survey. There will be a workshop on this topic at Melbourne.

Anniversaries

Forthcoming anniversaries in 2023 include 75 years for the IUCr and the journals, 40 years for *Acta C* and 30 years for *Acta D*. High-profile articles were commissioned for the 50th anniversary of the journals. It is proposed to concentrate on the last 25 years this time. All Main Editors are asked to go through the archives and put together a list of their most important papers by the end of May. Andrew Allen will write an editorial for the journals and the *Newsletter*. It would be good to have this ready for the Congress.

In addition, *IUCrJ* will be 10 years old in 2024, and *JSR* will be 30.

11. OUTREACH AND EDUCATION

Michele Zema gave an overview of IUCr outreach activities, emphasising opportunities for the journals to get involved and take advantage of the capacity building being undertaken.

AfCA will be proposed as a regional associate of the IUCr in Melbourne. This will be celebrated with an AfCA-IUCr virtual collection, with Guest Editors Susan Bourne, Delia Haynes and Michele Zema. Invitations have been sent out to over 700 potential authors. Single-crystal diffraction research is important in the region, so it is expected that many of the articles will be published in *Acta C* or *E*, or *IUCrData*.

2023 is the Year of Basic Science for Sustainable Development and also the Year of Mineralogy. There will be a special mineralogy microsymposium at the Congress. Michele will use his contacts to try to make sure the journals benefit from these years, including by sharing information on the journals with the many partner organisations involved.

The LAAAMP initiative was described. It is hoped to obtain papers from people who obtain grants for training at synchrotrons and who attend synchrotron schools. It would be good to have a Main or Managing Editor make a presentation at schools, describing the journals and answering students' questions. LAAAMP is also a main partner in the African Light Source, giving high visibility to the IUCr, but we have to make sure this leads to papers being published in our journals.

The X-Tech Lab in Benin could generate papers for the journals. Michele is also involved in two other initiatives, the Mexican Light Source and the Greater Caribbean Light Source. He is also trying to get a slot at the SESAME users meeting in May to showcase how we can support their research with our journals.

12. ANY OTHER BUSINESS

In his closing remarks, Andrew Allen expressed his enormous thanks to everyone for attending, saying that the discussions at the meeting had provided useful ideas that could be put into action. He stressed the importance of communication with the Editorial Boards and Commissioning Editors over the coming months. He also asked Main Editors present to pass on his gratitude and appreciation to all of our Main and Co-editors for all that they do.

13. DATE OF NEXT MEETING

There will be an in-person meeting in association with the Congress in Melbourne from 13:00 to 17:00 on August 23 2023, the first full day of the Congress. There will also be an Open Commission on Journals meeting from 12:00 to 13:00 on 24 August. For 2024, we plan an in-person JMB meeting in Chester in spring (to coincide with the IUCr Spring Finance Committee meeting).

JOURNAL ACTION PLANS

Journal action plan – *Acta A*

- Aim to improve the quality, increase the number of submissions and improve the impact of the journal.
- Previously, there has been a mismatch between aspirations and resources – revise plan so it is executable with current resources.
- Commission short (4-5 pages) ‘best practice’ or ‘how to’ articles from high-level authors. These should be in areas the journal wants to encourage submissions from. A template would be provided to the author. These articles will hopefully help increase the impact factor as well as defining the scope of the journal.
- Relevance to structural science is a challenge regarding the quality of submissions as some papers tend to be very mathematical. Trying to get authors to add details of a paper's context at a later stage has failed. Articles should be assessed in terms of scholarship, relevance, novelty and correctness. A pre-screening stage will be introduced into the submission process with articles judged on their scholarliness and relevance. Authors will get either a standard rejection letter or will be told that resubmission would be welcome after certain issues have been addressed. New text has already been worked on for the web page, *Notes for Authors* etc.
- A computational methods section will be introduced. Papers in different sections might be labelled by topic. It is hoped that this will help to attract papers.
- Work will be carried out to reduce review times.
- Assemble a virtual collection of articles on machine learning/AI in time for the Congress.

Journal action plan – *Acta B*

- Two of the Main Editors are due to retire. Replacements are needed and some overlap would be ideal.
- The experience of getting people to write feature/lead articles shows that it is difficult and not a good use of time. The journal will instead concentrate on the publication of special issues, one or two a year ideally. There was a special issue on non-ambient crystallography in 2014 that was well cited so may be worth revisiting.
- Commentaries are relatively easy to commission, are cited and the journal will continue with publishing these.
- The Crystal Growth section could be promoted more widely and the Co-editors for this section encouraged to either write or source/commission an article.
- Long publication times can be damaging to the reputation of the journal so ways to reduce handling time will be explored. In particular, ways to identify papers that have not had any action taken in a certain period of time will be considered.

Journal action plan – *Acta C*

- Two new Section Editors were appointed in 2022 with the aim of overlapping with the two Section Editors who will be retiring at Congress. This year of overlap has allowed a long and useful period of mentoring.
- The number of submissions is currently low so all future initiatives will address this issue.
- The journal is looking at starting a new section possibly centred on computational crystallography. In tandem with this, special issues may be a better way to determine which route to take. Ideas are: quantum crystallography, electron crystallography, knowledge-based discovery, powder diffraction and revisiting NMR crystallography.
- The scopes and keywords will be looked at in relation to those of Acta B. A new graphical scope will be created

to display the journal keywords.

- The review panel is key to helping reduce review times so it is important to keep it up to date. All current members have been contacted and asked if they wish to remain on the panel. Three new members were added recently.
- Pre-screening may be revisited in relation to reducing review times. It may also be needed if the range of topics in articles widens so as to better direct papers to the appropriate Co-editor.

Journal action plan – *Acta D*

- The number of submissions is key – currently the trend is in the wrong direction. Channels of communication with the Commissioning Editor will be opened.
- An editorial board meeting is being held soon. Members will be asked to come up with ideas for articles that could be commissioned and also to be ambassadors for the journal. The board needs to be refreshed and possible candidates are being identified.
- The review process needs to be speeded up. Co-editors will be advised of best practice. Work at the editorial office to identify where bottlenecks occur is welcome.

Journal action plan – *Acta E*

- The journal will receive an impact factor this year. It is expected that the number of submissions will increase as a result, particularly from China. The Editorial Board will be looked at with this in mind.
- The journal's teaching role will be maintained and strengthened. A currently running special issue on this area should be completed in the summer. The Section Editors will work with Michele Zema to link his outreach work with research that can be published in the journal.
- Special issues are being considered. It is expected that some papers from the AfCA initiative will be published in *Acta E*. A special issue linked to an ACA session is also being organised and will be published in collaboration with *Acta C*.
- A powder expert will be recruited as a Co-editor and a special issue will be explored with the aim of increasing the number of powder papers in the journal.
- Attracting more submissions reporting mineralogical and geological structures could be explored.

Journal action plan – *Acta F*

- The main challenges are to increase the number of submissions and to ensure the journal has an identity distinct from that of *Acta D*.
- In order to make the journal more distinct from *Acta D*, there will be a focus on short articles, and the editors will work to attract more short methods papers and reviews, expanding into more general scientific areas and reaching more young scientists. There could be a focus on sample preparation for all structural biology techniques, not just crystallization. Facilities papers (*e.g.* on crystallization, cryo-EM facilities) are also being solicited. The Section Editors will be more proactive in writing editorials.
- *Acta F* could have a role documenting unpublished PDB entries. pubBio could be used to prepare papers for prospective authors, especially those with access to open-access deals. Single-structure papers with little or no complementary data from other techniques are welcomed in *Acta F* while multi-structure articles that describe complementary experiments and discuss the underlying biology are better in *Acta D*.

- Some new Co-editors are needed. The Section Editors will reach out to the editorial board and involve them in ongoing discussions to determine future directions for the journal.

Journal action plan – JAC

- The overall aim is to increase impact and quality.
- Co-editors will be asked to identify interesting areas, and to talk to potential authors, encouraging them to submit.
- Work will be done to cut review times, perhaps by tweaking deadlines where appropriate for different stages of the review process.
- A special collection of previously published papers on machine learning will be put together. A guest editor has already been appointed. A joint special issue with *Acta A* (with commissioned papers) could also be explored.

Journal action plan – JSR

- Arrange a *JSR* editorial board meeting in May or June to explore Co-editor experiences, good and bad, with the journal, and to get them involved in initiating special issues and commissioning papers.
- Review and revise the scope of the journal. Use bullet points to show the areas covered by *JSR* (easier to access for potential authors) and include new areas (e.g. AI). Include the categories of papers that *JSR* publishes.
- Include a ‘this is my first submission’ button on submission pages. These authors can be given extra help if necessary during the review process, and publication of the paper will be celebrated on social media.
- Interactivity on social media will be improved.
- Adapt templates so that author institutions are included in the tweets sent out automatically when a paper goes online, e.g. @desy, @MAXIVLaboratory, for better coverage.
- Sponsor a new Synchrotron Radiation award to help publicise/highlight the journal. Possibly two awards - senior and young researcher. Nominations from synchrotrons. Award could be open access voucher?. Annually or biennially.
- Review the referee questionnaire list. Could some questions be removed or revised from the list that referees are asked to return?
- Look at ways to reduce review times and improve the chasing procedures.
- Appoint more Co-editors from major synchrotrons (e.g. Diamond, Sirius, SESAME, Canadian Light Source).
- Beamlines papers. Don't need to be novel, just technically sound and correct, i.e. to introduce the beamline. Standardize the format.
- Consider introducing a "raw data" option for X-ray spectroscopy and scattering methods.

Journal action plan – IUCrData

- The future direction of *IUCrData* needs to be considered. In the next few years, there will need to be Main and Co-editor appointments as Editorial Board appointed for the launch of the journal will have served a full term.
- More papers are needed for the Raw Data Letters section to improve the author tools that are being developed. Congress offers an ideal opportunity to advertise and promote the new section.
- The journal provides the opportunity to include new sections and these need to be identified in the next few

years. How *IUCrData* can be integrated with the other IUCr journals should also be kept in mind.

- *IUCrData* is currently indexed by Scopus and indexing by Clarivate will be looked at next.

Journal action plan – *IUCrJ*

- Need to refresh editorial board. Three out of seven Main Editors are due to retire. A slight change in direction might result after their replacements have been appointed.
- Measures to speed up publication will be explored.
- New subject areas for coverage should be identified.
- Richard Catlow is exploring commissioning a small number of high-level articles in crystal structure prediction. Further small, very select, high-level special issues could be considered (these might be precursors for special issues in other journals).
- Plans need to be made to celebrate the 10th anniversary of the journal.

Action items (in addition to those in journal action plans)

- Main Editors need to review journal scopes in time for Congress.
- *Acta C* and *E*: reply to Joe Reibenspies and Peter Corfield about proposal for special issue.
- Main Editors: be proactive in discussing items raised at the meeting with other Main Editors of your journal.
- Send draft reviewer guidelines to Main Editors for feedback.
- Explore options for including article titles in references.
- Investigate the possibility of multiple covers and making high-resolution covers more available.
- Commissioning Editors – Andrew Allen to work to clarify and communicate their role.
- Explore idea of putting journal-specific post-it notes on posters at meetings to solicit submissions in that area.
- Identify potential *JSR* Co-editors – Michele to suggest potential candidates at SESAME.
- Ask members of editorial boards about Congress attendance.
- Look at methods to make sure that referees read the supplementary material and review it along with the body of the paper, e.g. investigate adding supporting information to the review document.
- Develop tools to help authors decide where to submit, perhaps based on the abstract and/or keywords.
- Look into providing a web page where the scopes of all the journals are given.
- Explore possibilities for an online shop and a stall at Congress selling IUCr merchandise. The editors were enthusiastic about this and reported strong sales at other meetings.
- Design slides to be shown at the end of talks at meetings.
- Look into adding tick boxes to the IUCr journals' search results pages, to allow researchers to download batches of references in a format of their choice for adding to a bibliography.
- Main journal editors to be alerted to papers stuck in the system.
- Investigate changing how revised articles should be viewed by referees.
- Set a hard limit on the total number of papers that are active for a given Co-editor.

NOTES ON THE BREAKOUT MEETINGS

Biology group

Elsbeth Garman, Louise Jones, Mark van Raaij, Randy Read, Simon Glynn

Visiting for part of the breakouts: Andrea Sharpe, Andrew Allen, Hanna Dabkowska, Loes Kroon Batenburg, Peter Strickland

The number of submissions needs to increase

Articles can be commissioned by any of the Editors or Co-editors not just the Commissioning Editor. The Commissioning Editor, Section Editors and Managing Editors need to work together on commissioning so that everyone knows about plans for special issues and articles. The Commissioning Editor should also edit papers as appropriate and attend editorial board meetings to benefit from discussions with the Co-editors. When commissioning try to make the task less onerous for the person being asked, *e.g.* ask them and their team to contribute. Make invitations more personal *e.g.* ask how the field is developing from their perspective. Make it clear that papers will need to go through the review process.

The difference between Acta D and Acta F

Both journals cover any aspect of structural biology but *Acta F* should have shorter papers. For structure papers, *Acta D* papers should have more information on the biology and complementary experiments (*e.g.* biochemistry, other complementary techniques). *Acta F* papers need less (or none) of this extra information.

Ideas for Acta F

Acta F could document database entries and provide somewhere for unpublished PDB entries to be published and citable. publBio could be used to prepare papers for prospective authors. Should impact matter if the structure is scientifically sound? Could articles be about the same proteins under different conditions or from different organisms? Target people from institutions with OA deals with Wiley so that they do not need to pay for open access.

Sample preparation methods for all structural biology techniques, not just crystallization, could be published. Tips and tricks for preparing samples and solving your structure should be encouraged.

Negative results - things that didn't work, things that didn't get finished - could be included.

Commission short how-to papers on standard protocols (Elsbeth has promised to write one) and more general topics of relevance to structural biologists *e.g.* how to deposit your raw data (commissioned from Loes), how to review a paper, how to present a poster (Elsbeth), how to use *PyMOL* (if Schrodinger not able to produce a full paper), how to use AI, best practice articles.

Publish short computer programs and reviews of facilities (not beamlines).

Target early career researchers - *Acta F* would like to attract younger authors.

Rewrite the scope for *Acta F*.

Areas of expansion and new Co-editors

New Co-editors need to be recruited for both journals as many have reached the end of their term. It is possible to ask some people to stay on. For *Acta F*, new Co-editors could have an influence on how the journal develops. Ideas for new Co-editors on both journals were discussed.

Areas for expansion where new Co-editors are needed include cryo-EM and AI. If *AlphaFold2* (or similar) has been used

in a paper we need to publish biology data as well. Authors should say if AI has been used.

Reviewing

Provide Co-editors with training and guidance, including how supporting information is processed. Make sure the referees look at any supporting information and add supporting information to the review PDF if appropriate (*e.g.* validation reports). Look at the questions to referees to see if they could be improved. Make it clear to authors what happens to supporting information. Any invited articles also need to be reviewed rigorously. Should the journals consider open reviewing? Possibly arrange a workshop on reviewing at the Congress.

Data

Make it easy for authors to provide data for structures and make sure Co-editors know about the data. Encourage raw data deposition and investigate how many papers have raw data deposited (let Loes know the results).

Publicity

Co-editors should act as ambassadors, especially at meetings. At poster sessions, encourage editors to highlight interesting posters using stickers saying that they would be interested to see the work in the journal.

Social media is being used to promote the journals and *Acta F* has a Mastodon account. Should *Acta D* have one? The cover images used for Twitter need to be improved. A gallery of cover images would be welcomed.

To promote the wider scope of the journals, downplay *Acta Crystallographica* (use subtitles instead).

Chemistry group

Sandy Blake, Paul Raithby, Sean Parkin, Bill Harrison and Loos Kroon-Batenburg with Chester staff Amanda Berry, Sean Conway and Gillian Holmes. Visiting: Andrew Allen, Hanna Dabkowska, Peter Strickland, Michele Zema, Mike Hoyland

Scopes, keywords and choice of journal

The Chemistry journals (*Acta B*, *C* and *E*, and *IUCrData*) have the problem that previously there was a perceived hierarchical relationship between *B*, *C* and *E*, rather than them having complementary and distinct roles.

Currently, *Acta C* is being squeezed on one side by *Acta B*, which publishes more complex crystallographic studies, and *Acta E*, on the other side, which is now publishing multistructure papers with some crystallographic discussion.

The scopes of the chemistry journals will be looked at after the meeting to see if they need to be adjusted to both better define the current status of the journals and make a distinction between them, particularly between *Acta B* and *Acta C*. It is hoped to remove any confusion.

Acta B has a graphic representation of the scope and keywords (made about 10 years ago) that is still relevant. *Acta C* intends to produce something similar. *Acta E* and *IUCrData* have clear enough identities and don't think a graphic is needed. *Acta E* has the possibility of a new role aligned with IUCr outreach. The journal is also one of the main routes by which young researchers can gain experience of the journals.

Some authors know exactly where to submit their articles but some may need some direction. Some ideas to help with this: (i) a Venn-diagram-type image that would overlap B/C/E so that you could see the areas of commonality but also

where the journals differ. (ii) An uploaded abstract could be used to suggest which is the most appropriate journal (AI assisted). (iii) A web page for new authors that would direct them to the appropriate journal either using an abstract or keywords. (iv) A page devoted to the IUCr Chemistry journals presenting scopes and with links through to the journals. We have considered subject portals in the past.

Authors should be allowed to make their own choice of journal and if a paper is deemed to be suitable for a particular journal then it should not be moved.

The possibility of title changes was discussed, as was the possibility of merging journals, as there are probably too many journals covering similar areas. At the moment, under the present subscription model, such changes would not be possible. The landscape will probably change in the next 5-10 years, whereupon the structure of the suite of journals can be revisited.

Special issues and highly-cited articles

Special issues are a way of keeping a steady flow of papers and are generally cited above the background.

The CCDC want to do a structure-prediction special issue for *Acta B* and this will be ready shortly. This is the blind test and has been published in the journal previously. Richard Catlow is interested in a structure prediction set of papers (special issue) for *IUCrJ*. This could be small and very high level. The theme could then be developed in the other journals. *Acta C* was thinking of taking the results of the blind test and doing a special issue on the applications of the blind test. *Acta B* previously did a special issue around one of the blind tests on structure prediction.

A special issue for Africa is being organised by Michele Zema, Susan Bourne and Delia Haynes. Over 700 invites have been sent out. The areas covered will encompass all of crystallography so the special issue will not be specific to one journal, though it is envisioned that there will be a lot of single-crystal work, so *Acta C*, *Acta E* and *IUCrData* may be the main beneficiaries.

Another collaboration between *Acta C* and *Acta E* that is upcoming is a special issue arising from a session at the 2023 ACA Baltimore meeting on "Exploring Intermolecular Forces and Interactions" organised by Joe Reibenspies and Peter Corfield. The IUCr is sponsoring a student speaker and will cover the publication cost of a follow-up article in *Acta E*. The Editorial office will contact the organisers shortly to see how this is going to develop and to get actively involved. It could be a good model for capturing sessions at future meetings. The submissions will need to be research articles of good enough quality for IUCr journals. Cross-journal special issues face the problem of who is going to take overall responsibility for handling so this needs to be considered carefully.

Acta C is considering a special issue/article on electron crystallography (*Acta B* had a special issue on this in 2019) as one of the Co-editors is involved with the commercial side of this topic. The journal is also looking at a set of papers on quantum crystallography, as one of the Main Editors is familiar with this field, looking at practical methods so as not to clash with the *Acta B* special issue on the same topic from 2021.

Acta E has a teaching special issue that is doing well and is nearly finished. It would be a good idea to carry on with this topic, adding to it every year or two.

Best-practice articles usually attract citations and would thus be a way of sustaining impact factor.

Regarding commissioning of reviews and lead articles, it might be a good idea to make it clear when contacting a research group leader that that the involvement of young members of the group is encouraged. This could lead to the involvement of early researchers who would have more time to devote to such work.

Bo Brummerstedt Iversen produced a list of special issues for a recent *Acta B* Main Editor meeting. This will be looked at to see which are appropriate for *Acta C* and *Acta B*.

New sections and new areas to consider

The *Acta B* Crystal Growth section has attracted a small number of papers, possibly because the competition in this field is already well established. The assigned Co-editors could be asked to commission articles to get the section moving.

Acta C needs to be considered carefully and needs to find its own niche. The computational side of crystallography would be a good area to expand into. This would need to be backed up with new appointments. Quantum crystallography/Hirshfeld atom refinement is also a possibility. *Acta B* had a special issue on Quantum crystallography and the issue could be analysed to see what worked. The chemistry field is already well populated and *Acta C* is not seen as a chemistry journal within that community.

Promotion and meetings

We should be more specific in our use of Co-editors attending conferences. They should be sent promotional material and they could be asked to incorporate a one-panel overhead into any talk they give, which could be either journal specific or for IUCr journals in general.

An application will be made for *IUCrData* for coverage by Clarivate. It is already covered by Scopus. Submissions have decreased recently but it is hoped that the journal will find its feet and thrive with the addition of new sections in the coming years.

Learned society meetings are probably the most focused meetings to attend. RSC, ACS, ACA and the regional affiliates are others to consider. It may be more useful to know which members of the editorial boards are going to which meetings and support them with information and materials. Also we may have more presence on Wiley stands in future which would provide focus and a meeting place without having a full stand. However, an IUCr stand is still seen as the best focus at a meeting.

Review times

The submission system is working well. Main editors would like alerts when there are delays with articles.

A text message could be sent to a Co-editor when a paper is submitted; this would be opt-in.

Reducing review times may be helped by: (i) PROPHY, (ii) letting Co-editors be aware they are slow compared to the journal average, (iii) review panel and (iv) pre-screening. Delayed papers can be reputationally damaging and need to be identified. There could be a page that is more sophisticated than the current "delayed papers" page to alert Main Editors to problems. But the preferred method of alerting Main Editors to delays would be an email at the appropriate time.

Pre-screening has not been used previously on *Acta C* but might be considered again when the Editorial Board is renewed after Congress. It is a way of reducing review times and also directing articles effectively to appropriate Co-editors if the content of articles in the journal expands.

Open-access charge

The open-access charge on *Acta E* might be a little high at 500 USD per article, especially if only a single structure is reported. It might be worth considering a sliding scale, the open-access charge increasing with the number of structures reported, with a cap on the charge. There is precedent for this with other publishers.

Cover illustrations

If there is time in the production cycle, it might be worth asking authors to create a graphic for the cover, especially if the paper does not contain anything that would be especially suited to a cover image. Authors could also be asked to submit a

cover style image on submission.

Editorial boards

The Editorial Boards should increase their Co-editor presence from Asia.

Acta B is very happy with the current spread of gender/geography/expertise on its board, but the two new Section Editors should have the opportunity to reassess this matter. *Acta C* has had a rolling recruitment in recent years so has only needed to replace a few in the run up to Congress. The correct spread in terms of gender and geography is difficult to achieve. *Acta E* will be replacing quite a few of the Co-editors. Also it will be reindexed with Clarivate this summer and is expecting to see an increase in the number of submissions and so will use the opportunity to strengthen the board. It is expected that Chinese authors will return as students need an impact factor to graduate and *Acta E* will now supply this.

IUCrData will be nine years old next year, so an overhaul of the board is imminent. This will go hand-in-hand with discussions on what the future and direction of the journal is likely to be, and will determine appropriate appointments. Raw Data Letters is the new section in *IUCrData* and has papers that would be appropriate for *JAC* so it's had a strong start.

Materials, Methods and Instrumentation group

Simon Billinge, Janos Hadju, Kristina Kvashnina and Thomas Proffen, with Chester staff Nicola Ashcroft, Lisa Stephenson and Tony Weight

Breakout 1

Editorial Board Zoom meetings were discussed. The main concerns for both *Acta A* and *JAC* Co-editors was the difficulty in getting reviews. Automatic reminder emails are now being sent to reviewers a few days before their review is due, which might help.

Co-editors could be asked to provide suggestions for good articles to commission. The Editorial Office could take responsibility for sending out reminders to authors once they know which papers have been commissioned and when those articles are due by.

All three journals have already published a number of papers featuring AI/machine learning; these could form a themed collection, along with an Editorial or Foreword, to be publicised at the Congress.

Janos reported problems with invitations to reviewers being rejected as spam, possibly because of the links in the emails used.

It was noted that it is inconvenient that second reviews (i.e. of revised papers) are only found within emails and are not stored in the submission system in a way in which they can be attached easily to an email to the author.

It is possible that not all Co-editors are aware that there is an option to transfer a paper to another IUCr journal, so it would be useful to remind them that there is a mechanism for this. It might also be worthwhile to remind Co-editors about potential conflict of interest problems if they were to handle papers from authors within their own department, or to choose reviewers who have worked closely with or are in the same department as one of the authors. There is a mechanism within the submission system to help to prevent such situations arising, but Lisa noted that it does not always work.

Ways to increase submissions to the journals were discussed. Kristina said that if she receives a thorough review for an article she often suggests to the reviewer that the journal would welcome an article from them in the future when she

writes to thank them for their review. MDPI journals offer 'your next paper free' to people who have reviewed four papers.

Reducing the time taken for an initial decision could be useful too, i.e. providing a quick yes or no decision within a week. This would fit with *Acta A*'s proposal to introduce pre-screening for all papers.

Encouraging shorter papers might also help to increase submissions.

Different ways in which the journals select the cover image were discussed. Janos suggested choosing more than one cover image and providing a 'carousel' of images on the web page, each showing one of the covers for a few seconds, and each linking to the relevant paper. The Editorial staff were reminded that some institutions have graphics designers who could help with designing a cover image. Journal covers are often displayed in foyers, corridors etc. and so act as powerful free publicity for the journals.

Breakout 2

For this session, the group was joined by Andrew Allen and Peter Strickland.

There was further discussion of papers involving AI. Simon asked whether a new section of the journals might be needed for these. Andrew said that this could be done if the section would attract enough papers. It was agreed that there was a strong case for these papers in each of the three journals.

Janos asked if we had too many journals at present and whether they could be merged into one. Peter explained that a new journal would not have an impact factor for the first four years, so would be unattractive to authors. However, once the transition to open access was complete for all journals, the separate roles of each journal could be reconsidered. The level of subscriptions that each journal has, which can depend on the journal's history, is a barrier to merging them at present.

Simon wondered if we were missing out on papers by not having a 'computational methods' journal, but thought that we could launch such a section in *Acta A*.

It was thought that the different roles of each journal could make it difficult for authors to choose which journal to submit to. A web page showing all the scopes (and impact factors) together might be helpful.

Breakout 3

The group was joined by Michele Zema for this session.

It was noted that authors still consider the impact factor of a journal as very important. Researchers might choose a journal for a particular paper using Web of Science or SCImago, but students sometimes just use a Google search term such as 'high impact chemistry journal'.

Thomas said that it can be difficult to persuade fellow authors to send a paper to an IUCr journal if they haven't heard of the IUCr. Simon thought that having the word 'crystallography' in the names of most of our journals could be unhelpful and might discourage submissions from some authors, who could view the journals as too specialised.

New sections of a journal or new areas that it covers might usefully be publicised briefly in the many emails that we already send out to authors and referees during the submission and review process.

Transferring unsuitable papers from a high-impact journal to a lower-impact or new journal from the same 'stable' can raise awareness of the second journal (a strategy often used by Nature).

Kristina suggested that we might have a tick box for new authors to use when submitting an article to indicate that it was their first paper. The Co-editor would then know that they might need a bit more help and guidance than other authors, and social media could be used to promote their paper when it is published, so providing a welcoming overall experience

to new researchers.

Michele mentioned that his outreach work meant that he had access to lists of participants from meetings, workshops etc. It was agreed that these would be useful for journals promotion as long as the participants had agreed that they could be contacted. Janos said that in cases where bulk emails were not suitable a personal approach could be very effective.