Acta B/C/E meeting

Euroforum Infantes, San Lorenzo de El Escorial, Spain

20 August, 09:00-11:00, Auditorio02

CHAIR: Carol Brock

Attendees: Acta B/C/E Editors and Co-editors

IUCr staff attending: Jill Bradshaw, Sean Conway, Gillian Holmes

1. GENERAL

Carol introduced the meeting by noting the changes to the Section Editors for both Acta B and Acta E. Carol Brock is retiring as Section Editor for Acta B and will be replaced by Sander van Smaalen; on Acta E Jim Simpson is stepping down as Section Editor (but will stay on as a `forensic editor') and is being replaced by Helen Stoeckli-Evans and Edward Tiekink.

Carol then gave a presentation on Acta B, noting that the primary focus of the journal was on structure. However, an Acta B paper should be more than just a structure unless the structure is very complicated. Acta B covers a broad subject area, including phase transitions, electron-density determinations, polymorphism etc., and is distinguished from Acta C by the scope of the papers. Acta B papers are of lasting importance and one of the strengths of the journal is that it allows the publication of techniques that other journals do not allow. There has been a trend over recent years for papers to be longer with increased scope and depth. This could be a problem as they appear intimidating and may discourage potential authors whose papers are not as broad or deep. There is a trend for increased amounts of supplementary material and, worryingly, fewer molecular papers. The strengths of the journal include its excellent reputation for quality, its thorough refereeing and editing, its software expertise, which allows structures to be checked for self-consistency, and the generosity of the people involved with the journal. The importance of the referees cannot be overstated.

However, the journal currently faces challenges, not least due to the difficult economic climate and the worldwide emphasis on self-promotion, which make impact factors very important. There is also the distinction made by non-crystallographers between chemistry and crystallography, which is viewed as a `non-science' supporting technique in the US. Some competing journals, especially in the molecular area, require much less especially in the area of crystallographic competency. It is perceived that publication in the two major competitors of Acta B, Crystal Growth and Design (ACS) and CrystEngComm (RSC), is more favourable for grant applications. This is independent of the impact factor although these journals do have a higher impact factor than B. They also require less information, e.g. structure factors are not a requirement. These are problems we cannot ignore. The conundrum is that the journal exists to serve the IUCr, reflecting the attitudes and skills of crystallographers with emphasis on quality, standards and education. However, the journal must remain economically viable in a difficult and uncertain economic situation. Unfortunately, our competitors do not seem to operate in the same way so we need to look at how to make sure libraries still subscribe to the journal. Carol encouraged Co-editors to help the IUCr by accessing the journals online via their libraries as the number of logins are counted.

Carol noted that she read all the proofs and one of the strengths of Acta is careful editing. She said she always tried to help authors by writing comments in a way that if she were receiving them she wouldn't be annoyed or offended. We need to help authors and keep them happy as without authors there is no journal.

In summary, Carol commented that the IUCr journals are carefully edited journals that report excellent science and are supported by a generous, skilled community. However, there are a number of perceptions we need to fight – one being that crystallography is just about the solution of crystal structures. It is so much more than that. Also there is the impression among the community that Acta referees and Co-editors are trying to enforce unrealistic standards. Maybe this is true but it is something to consider for the future of the journals.

Carol then reported that Sander van Smaalen was to be the new Section Editor for Acta B. He has handled many papers reporting molecular crystallography and has published many papers in Acta journals, especially in Acta B. Carol then finished by thanking the Chester staff, especially Jill Bradshaw.

Sandy Blake commented on the issue of self-promotion and the fact that everyone in the UK has to write an impact statement. As everyone has to do this it has become institutionalized and so is worthless but still people are required to do it well. Jim Simpson agreed that self-promotion is a requirement that we all feel uncomfortable with and said the

situation is the same on the other side of the world. It was an absolute requirement of academic life now but most people are uncomfortable having to push themselves forward to in order to promote their departments and universities.

2. VALIDATION

Sandy Blake gave a presentation on data validation which will be made available online. A discussion followed including weighting schemes, structure-factor checks, handling disorder, data completeness and Hirshfeld alerts. Carol Brock ended this by recommending that all B, C and E Co-editors make a rotatable structure that displays ellipsoids as it was a much easier way of spotting problems. Problems must exist in other structural journals that they do not even want to know about. The question was did this matter. If it was a missing water molecule, definitely; the wrong weighting scheme, maybe not so much. These were judgement calls but what matters to the crystallography community differs from what matters to the chemistry community. Carol noted that Jack Dunitz had said that half of what was published in the scientific literature is wrong. Acta journals can sometimes be a bit compulsive about making sure nothing is wrong.

3. JOURNAL IDENTITY

Jim Simpson raised the issue of the relationship between the journals. Jim said that Acta E had now found its niche, publishing over 4000 structures a year, largely due to an effective team of Co-editors. Since the journal changed to the shorter format, it had established itself as a simple, straightforward way of presenting a paper and the situation was likely to improve. He felt that the problem was the C/B interface. To an author, it seems that the bar on C is being raised but B is staying where it is (*i.e.* papers are submitted to Acta C rather than B) - do they collide? Several people had mentioned this to him.

Carol said that with few exceptions, there was not a major problem of papers that used to go to B now being published in C. There would always be borderline cases but this was not cause for concern as far as she is aware. Ultimately it is the author who chooses where to submit their paper. Sandy Blake said that C was not in competition with B. Acta B papers are longer and becoming more so, and tended to contain more structures and/or discussion. The papers were getting fewer in number as they took longer to write. He thought there was perhaps more concern about the C/E border as it did not take much effort to turn an E article into a C article.

Elena Boldyreva felt that the appearance of E had been of benefit to C. Acta C contained papers of different length and allowed more choice of titles. She commented that interesting titles and subtitles help people find our journals in a sea of publications. However, people are forced to publish in other journals because of the impact factor and *h* index requirements for grants. She felt that there were not enough B submissions as not many people were able to produce such papers. If we published more special issues on hot topics such as crystallographic aspects of crystal engineering, that would help the journal become more attractive to authors. She felt it would increase the impact factor if educational reviews were included in each issue for example. One drawback of publishing in Acta B is the length of time from submission to review, which is too long. Authors will publish hot topics in high-impact rapid-publication journals rather than journals such as Acta B which have publication times of 4-5 months. She also felt that it was necessary to be more pro-active in inviting authors to publish in B and selecting topics for future reviews. Elena reported that her department had an informal requirement that students should publish at least one structure in Acta C to get a high grade. Acta C and Chester were used as a free service to check work! She recommended that we should advertise this and encourage people to use it for qualification purposes. Elena also commented that the Executive Committee was worried about the current status of the journals. Acta B is a great journal but the submission rate is currently low and the gap could possibly be filled with reviews and educational papers. The journals should be more active and more smart.

In response to Elena's comments Carol noted that there had been a number of suggestions over the years about what Acta B should do and that she had learnt from early on that it does not work to play someone else's game – that was worse than doing nothing at all. We need to remember our identity and our integrity but it was agreed that we do need to monitor the situation. On the subject of publication times Carol noted that it was difficult to maintain quality without spending the time. We do not have to win the race, just not lose. Special issues had always been a problem in that it has been difficult finding people to agree to oversee them. Recent plans for two special issues have faltered. An update of the special issue on databases failed as we could not get papers from the CSD or the PDB. A second proposed special issue on crystal engineering also failed because of authors' other commitments not allowing them to devote enough time to organising the issue. As for publishing reviews it had been a policy decision of the IUCr not to publish reviews. However, feature articles could function as reviews but it was preferable if there was at least some new work reported.

Phil Fanwick said that part of the conundrum was that a journal needs to serve the needs of authors and readers. However, these needs do not always overlap. Readership is broader than authorship and impact factors are important for authors rather than readers. It was not easy to reconcile how to support the author while meeting the needs of the reader.

4. PUBLICATION OF DATA

It was felt that cell parameter s.u.s were still a significant problem, with most people reporting the mostly very small values given from the CCD data. If more realistic values were used people would question if the diffractometer was misaligned. Ilia Guzei reported that a Monte Carlo approximation gives a better estimation although the s.u.s were still a bit low. He had tested this on around 450 good data sets.

Matthias Zeller said he would like to see the twin ratio in the table for twinned structures. This would also avoid the need to report it in the abstract. Matthias Weil commented this would require new data names. Carol Brock and Ton Spek commented that this was work in (slow) progress.