

Acta C meeting

Euroforum Infantes, San Lorenzo de El Escorial, Spain

20 August, 15:00-18:00, Sala11 (Editors are encouraged to join the Acta B/C/E and C/E meetings before this meeting)

CHAIR: Sandy Blake

Attendees: Ricardo Baggio, Andrew Bond, Jean-Claude Daran, Mark Elsegood, Larry Falvello, Phillip Fanwick, George Ferguson, Ilia Guzei, Maciej Kubicki, Vratislav Langer, Bernard Santasiero, Ton Spek, Amber Thompson, Dmitry Yufit

IUCr staff attending: Sean Conway

TRAINING

Sandy Blake presented a short talk covering important points related to the handling of Section C papers.

GENERAL DISCUSSION

- (i) Packing diagrams in Mercury sometimes did not relate to what was intended to be shown. No-one was aware of a solution to this.
- (ii) Co-editors sometimes ask for information like geometry ranges that are available in the CSD but should be aware that not all authors have access. Co-editors can provide information like this for authors without CSD access but should not do so regularly.
- (iii) Compound names were still checked and created in Chester and Co-editors do not need to spend too much time on this aspect of a paper.
- (iv) Zero-tolerance should be applied in cases where the English is bad and one/some of the authors might be English speakers.
- (v) Symmetry codes were sometimes seen as a barrier for authors, but if these are used then they should be correct. Intermolecular discussions will require the use of symmetry codes so inclusion of symmetry codes cannot be avoided.
- (vi) It might be useful if there was an online location where readers could leave comments on the journal. Letters to the Editor can be published in Section C.
- (vii) If e-mail addresses are supplied during the submission process then all authors are notified about the submission.
- (viii) There was a discussion of s.u. values on cell parameters. The software cell parameters might be reported, together with the software they came out of and the time of collection. We need to think carefully about any changes we make to requirements as what we do affects other non-IUCr journals. The impact of the cell parameters on geometry is very small, unless you go to the second decimal place, and chemical discussions are still valid.
- (ix) .ins and .hkl files might be included in the Co-editor .zip file. Could some automatic descriptive text for H-atom treatment be generated automatically from the CIF? Chester will look into the fact that some .zip files also contain files from the tracking submission.
- (x) The Section Editor correction stage might involve the Co-editor again because sometimes the Section Editor goes over items that have already been discussed by the Co-editor with the author and it looks bad both for the Co-editor and for the journal. Acceptance might be delayed until the Section Editor has seen the proofs or until the Co-editor has had a chance to consider the Section Editor comments. Co-editors felt some form of unification of comments was needed and a mechanism decided upon.
- (xi) The refinement instruction file wording in Notes for Authors was thought to be appropriate.

JOURNAL DEVELOPMENT

There was a discussion about how to attract more papers to the journal, and papers from the chemistry and pharmaceutical fields were seen as targets; Journal of Natural Products and Medicinal Chemistry Letters have structural papers than fit with the Acta C profile. We should not relax our standards but continue to be as helpful to authors as

reasonably possible. pubCIF should be more widely publicised. The information and policy in Notes for Authors about previously published structures also needs to be more widely publicised. We need to emphasise that we are willing to handle papers on difficult structures. New classes of compounds are also good papers to aim for.

PUBLICATION SPEED

One of the biggest problems affecting publication speed is finding referees and getting back reports. Various solutions were discussed, such as a review board or a database of referees. It might be useful to ask retiring Co-editors if they have any names of good referees to pass on. Also, getting authors to suggest referees during the submission process might be useful if they can be encouraged to do this. A better way of finding out if a referee is going to handle a paper or not would be useful and would avoid unnecessary delays.

Other journals offer rewards for referees, such as free access to the journal for a limited period. Co-editors should use thank-you letters; these can be personalised by contacting the Chester office. Some Co-editors find it useful to send a message to potential referees outside the system before a formal invitation is sent.

VIRTUAL SPECIAL ISSUES

A virtual special issue on polymorphism is planned for the end of 2011. This was thought to be a good idea. "Difficult techniques" was suggested as a possible future issue.

CONSISTENCY OF STANDARDS IN REVIEWING

Borderline cases sometimes cause problems, especially where the referee thinks the paper is acceptable. The Co-editor has the final decision and needs to be ruthless early on to avoid carrying on with a paper that is not going anywhere. The Section Editor can be approached if the Co-editor is unsure of how to proceed.

NOTES FOR AUTHORS

The mention of "empirical" with regard to "absorption correction" needs to be altered to match the core CIF dictionary.

EDITING GUIDELINES

Editing guidelines and a brief checklist are available for Section E Co-editors (see Appendix E). Similar documentation would be useful for Section C Co-editors.

DFT CALCULATIONS

The discussion of DFT calculations can sometimes be just padding and it is difficult to find experts in this field.

JOURNAL PROMOTION AND SPONSORSHIP

Co-editors were given a copy of the latest leaflet promoting Section C and were asked to return any comments or ideas for improvement to Chester.

The meeting was joined by the IUCr President Sine Larsen who asked the Co-editors present to consider ways that the journals might celebrate the upcoming International Year of Crystallography (IYCr2013). A collection of historically interesting papers was suggested.