

Acta C/E meeting

Euroforum Infantes, San Lorenzo de El Escorial, Spain

20 August, 11:30-13:00, Auditorio02

CHAIR: Jim Simpson

Attendees: Acta C/E Editors and Co-editors

IUCr staff attending: Sean Conway, Gillian Holmes

SUBMISSION AND REVIEW

It was felt that e-mails sent to authors via the status system would be clearer if any CIF formatting (e.g. bold and italic mark-up) was removed. It would be useful if all e-mails to authors could be accessible from the website, giving a complete record.

PREVIOUSLY PUBLISHED STRUCTURES

The current Notes for Authors wording on previously published structures, even though it differs between the two journals, was thought to be appropriate.

POOR QUALITY PAPERS

This does not only relate to poor language but also to crystallographic problems. Co-editors should attempt to improve papers but not to the extent that they are effectively rewriting the paper. Early assessment will save time later and Co-editors should ask the Section Editor for advice if they are unsure. For Acta E, the Comment can be removed as a final step if this is all that hinders publication.

ADDITIONAL INFORMATION

All authors of a paper are sent messages when a paper has been submitted alerting them to the submission if e-mail addresses have been supplied.

Having new CIF datanames for where the data were collected and by whom, and who solved and refined the structure and prepared the CIF was thought to be a good idea and that the person who collected the data should be included as an author or in the acknowledgements. The CSD ask for an e-mail address of the crystallographer connected with the data.

Even though publication of an Acta E paper without a Comment is allowed, a short and informative Comment is desirable. This cannot be enforced as Notes for Authors allows publication without a Comment and authors should not be given conflicting advice.

The statement in the Notes for Authors

"Co-editors may request any additional experimental data or material they feel necessary to complete a full review of the article."

was thought to be good enough. .res files are now included in the CIF when supplied.

Completeness is not well reported at present. Completeness per shell might be included. PLATON calculates this and it might be added but we normally do not require items that SHELXL does not produce. Including the structure factors in the CIF would get over a lot of validation problems though it does produce big files which might cause publication problems.

Problems associated with twinning and the use of SQUEEZE were discussed.

FIGURES AND SCHEMES

The quality of the artwork in review PDFs is sometimes poor even if the submitted artwork is of good quality. Chester is

aware of this problem. Stereo diagrams are no longer seen as having much value.

MARK UP OF CHEMICAL CONTENT

Initiatives to create chemical structural diagrams from the information in the CIF and the generation of chemical connectivity files for publication online as supporting material were outlined.