

# Acta E meeting

**Euroforum Infantes, San Lorenzo de El Escorial, Spain**

20 August, 15:00-18:00, Auditorio02

**CHAIR: Jim Simpson**

Attendees: Dmitry Albov, Ricardo Baggio, Kumar Biradha, David Brown, Vladimir Chernyshev, Jean-Claude Daran, Parthasarathi Dastidar, Laszlo Fabian, Jan Fabry, Karla Fejfarova, John Gallagher, Maria Gdaniec, Tayur N. Guru Row, Ken Haller, Owen Johnson, Biserka Kojic-Prodic, Sergey Lindeman, Gary Nichol, Masood Parvez, Georgina Rosair, Victor Rybakov, Helen Stoeckli-Evans, Edward Tiekink, Arie van der Lee, Matthias Weil, Matthias Zeller

IUCr staff attending: Gillian Holmes

## INTRODUCTION

Jim Simpson opened the meeting by reporting that he was retiring as a Section Editor and would be replaced by Helen Stoeckli-Evans and Edward Tiekink.

## EDITING GUIDELINES

Jim Simpson then gave a presentation on the “Acta E from Hell”, an invented paper including problems commonly encountered in Acta E submissions that was intended to illustrate the detailed editing guidelines circulated earlier in the year. He highlighted the various problems with this paper and detailed the changes that needed to be made at the review stage to make it suitable for publication. The powerpoint will be made available online.

Matthias Weil then gave details of specific requirements for metal-organic structures. The *Abstract* should include details of any disorder (including occupancies with s.u.s) along with details of special positions or symmetry (*PLATON* and *Mercury* are useful for this). Coordination numbers and polyhedra should also be given in the *Abstract*, supplemented by respective bond lengths in Table 1 (don't report symmetry-related distances; angles are normally of no great insight). Matthias commented that coordination numbers are a very good measure of the correctness of a metal, as are bond lengths. Crystallographic directions should be given in the *Abstract*. The crystal colour should be consistent between `publ_section_exptl_prep` and `exptl_crystal_colour`. If the colour itself seems wrong, it may be a warning sign that the metal is incorrect. Matthias then indicated possible problems with rare-earth metals and recommended re-refining structures with *PLATON* as a check. Other useful tools are *pubCIF* and *Mercury* and chemical intuition and knowledge. The powerpoint will be made available online.

David Brown recommended that anyone handling inorganic structures should do a bond-valence check as this technique supplies the crystal chemistry and gives warnings that can indicate an incorrect structure. He offered to put together some notes on this valuable tool.

A short discussion on the treatment of disorder followed. *SQUEEZE* should be used only as a last resort. *PLATON* is useful in the case of disorder as it does a complete analysis of the coordination and defines the complete polyhedron.

Jim commented that Co-editors should look more closely at the *Comment* section. They need to spend a little more time and effort to make sure that it is either tidied up or dispensed with altogether as we do not wish to present the readership with material that is not appropriate.

The problem of very quick and unimproved resubmission of poor articles was mentioned by Vladimir Chernyshev who suggested that authors should not be allowed to resubmit within a certain time limit. Some authors require rapid publication for their students and the time threat may be a good way of preventing this. Some authors, including experienced ones, are getting lazy and submit papers without adequate preparation. Jim Simpson said he could understand the frustration Co-editors felt. They could reject papers that came back in as bad a state and papers can be rejected without right of resubmission if it happens again (Co-editors should ask Chester who will consult the Section Editors if they require a paper to be permanently rejected). He commented that there are experienced authors who get students to write their papers. The senior authors do not check them and rely on Co-editors to tidy the paper up but this is not their job. Matthias Weil commented that it was difficult to set deadlines and that there have been cases of more or less identical papers being resubmitted months later. Co-editors were happy to help authors with their first submission but got angry when subsequent articles were just as bad. Matthias Zeller commented that he rejected papers if they were not done properly after the third revision and that if you consistently reject papers that are not up to standard, you get fewer of these problems.

The difference between rejection and withdrawal was discussed. Withdrawal could be more diplomatic and a slightly softer option. Authors can be invited to withdraw their paper but rejection is the Co-editor's option.

Ricardo Baggio picked up on Jim's comment in his "Acta E from Hell" presentation that the *Abstract* shouldn't be repeated in the *Comment*. He said that many authors don't realise that the *Abstract* is the core of the paper. Sometimes the Co-editor picks the good material from the *Comment* to put into the *Abstract*, leading to the situation where the *Abstract* is very similar to the *Comment*. Jim replied that in an Acta E paper, the *Abstract* is the primary vehicle of communicating the structure to readers. If minimal, authors should be given the opportunity to amend it, pointing out that if it is not suitable, they can adapt the *Comment*. David Brown noted that he finds it useful to recommend that authors look at published Acta E papers. Jim agreed that the mantra should be: "look at *Notes for Authors* and read some other E papers". Some authors have done neither and it shows!

## **REPORT OF SECTION E EDITORS MEETING**

Jim Simpson then reported that the Section Editors had met the week before in Chester. This had mainly been baton-changing as he was retiring. They had welcomed Helen and Edward to the team and had an interesting discussion on the role of Section Editors. He was also pleased to welcome a considerable cohort of new Co-editors to the team. They are in place and getting up to speed. There were sadly some retirees, including Jean-Claude Daran who was present at the JComm meeting. Jim thanked him and everyone else who was retiring or who had done so over the past couple of years for all their efforts, as without Co-editors, the journal would just not survive. The journal publishes over 4000 structures per year and he thanked everyone very much for all their time, effort and commitment.

## **JOURNAL GROWTH**

Jim reported that Acta E was still growing although this appeared to have reached a plateau. As we will be losing some experienced Co-editors, we will probably need to recruit some new ones soon. He therefore asked everyone to pass on their recommendations of any colleagues or friends to one of the Section Editors.

## **JOURNAL DEVELOPMENT**

It was not envisaged that there would be any major changes to the design of the journal over the next year or so but they were always open to comments and suggestions. Jim reiterated that if any of the Co-editors had problems or were unsure, they should ask the Section Editors as it was one of their tasks to provide support and feedback. Gary Nichol commented that he had been asked by several people why the ellipsoid plot is not part of the published paper. Matthias Weil replied that it was difficult to extract for polymeric structures and inorganics.

## **NOTES FOR AUTHORS**

Masood Parvez said he felt the use of SQUEEZE should be clarified. Matthias Weil proposed that a VRF should be required for SQUEEZE. Matthias Zeller suggested detailed instructions were needed regarding .fcf files and Sergey Lindeman commented that SQUEEZE was often used unnecessarily because the author could not handle the disorder and that it was easy to make mistakes with SQUEEZE. David Brown agreed that SQUEEZE should be a last resort and that its use should be justified. Authors should supply both the original and the SQUEEZED structure factors and include all solvents as far as they are known in the formula. Ken Haller said that if PLATON generates a file, we should require it and commented that you cannot go back from SQUEEZED structure factors.

## **PROMOTIONS**

The Acta E promotion leaflet was circulated.

## **SUMMARY**

In conclusion, Jim thanked everyone for coming and for all their work for the journal.