Information for (New) Co-editors

This presentation was used at the new co-editors induction meeting held during the IUCR Osaka Congress, August 2008.

It was rather quickly thrown together, but the contents may be useful as a general guide to co-editorial procedures

Tony Linden, September, 2008

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Topics

- Initial assessment of paper
- Selecting referees
- Time frame
- Co-editor vs Section Editor
- Things to check for
- Using Platon
- Requesting revisions
- Handling the revised paper
- Editing the final CIF

Notes for Authors

- Please make yourself thoroughly familiar with the Notes for Authors
- Authors should adhere to the NfA, but often do not read them
- Be familiar with journal style requirements, e.g. atom labels in figures do not have parentheses
- Read through the handbooks and other information supplied, e.g. the ‘useful links’ section of your co-editor home page

Initial assessment of paper

- If the structure is clearly wrong, the CIF is deficient, or…
- Abstract and Comment far too short and/or totally incomprehensible…
- Don't waste time on it and no need to use a referee at this stage
- Write a short, kind note to say paper rejected and give some of the reasons
- Acta E style papers sometimes submitted to C. Reject and say the format looks more appropriate for E or some other archival journal and they should submit there
- Rejected papers, if resubmitted, usually automatically come back to same co-editor
- If you get a note that a paper has been handled previously, you may need to contact other co-ed to ask why the paper was rejected
- Duplicated structures need to have a very substantial reason to be published again (e.g. much improved model or significant extension of earlier discussion - see Notes for Authors)

Selecting referees and time frame

- Use at least one referee initially
- People who are knowledgeable in the field, know the Acta requirements, are fair and who respond quickly are best
- If other results or chemistry reported, may need a specialist in that area
- Reports ideally within one week. If referee is not responding, try another quickly
- Referees often do not do a thorough job, e.g. they look only at the discussion, not at the nitty-gritty of the structure or correctness of numerical items in the paper. So you need to also cast a critical eye over the paper and make your own comments, as required

- Revisions within one month - better to request prompt action - but not immediate (authors should take time to think about their paper). If a deadline arrives, enquire if action can be expected soon, rather than waiting in silence.
- When more cycles of revision are needed, this can eat up time
- If not acceptable after two cycles, NfA allows you to reject. Your choice

Co-editor vs Section Editor

- Co-editor has full freedom to handle the paper as he chooses right up to the fully acceptable product.
- Section Editor reads proofs:
  Hopes nothing further needed.
  May ask for minor corrections or additional info from authors if something has been overlooked.
  These corrections dealt with by Sean Conway who contacts the authors if necessary. We don't usually send it back to a co-editor to arrange things, unless the whole paper needs serious work.
- My messages to Sean get sent automatically to handling co-ed. Meant as a learning aid so you see if you were not aware of a need or forgot something. It is a way to keep consistent standards.
- Author grievances: author should be directed to contact Section Editor.
- If you suspect deliberate manipulation of data (fraud), do not accuse authors of this, but advise the Section Editor. Some inexperienced people do things out of sheer ignorance.

Things to check for

- That the NfA are fully complied with.
- Abstract:
  - should summarize the key points made in the paper - not tell us that we are going to be told about something.
  - any symmetry elements in a molecule should be mentioned.
  - molecular formula stated, compound name if not in title.
  - no synthesis details or crystal data.
- Comment
  - Should tell a story - see Notes for Authors.
  - Intro to put chemistry and structure in perspective. Pointless if the structure does not relate to the intro topic. Any aims should be answered later on (often not).
  - Should be chemically and crystallographically logical
  - Should avoid over-analysing of barely significant interactions or ridiculous intramol C-H…X H-bonds (e.g. C-H and X-C are parallel).

Things to check for

- Check that symmetry codes are present in text for all symmetry related atoms mentioned, e.g. discussion of contacts, H-bonds.
- Also in figure captions.
- Atom labels should be beside the correct atom!
- Symmetry related atom labels in figures must have a symmetry code (superscript or other symbol is OK).
- In packing, the labels without sym. ops must correspond to the position of these atoms defined by the model.
- In packing, cell axes must be shown and labelled, omit H not involved in contacts.
- Must have a labelled ADP plot of the molecule or some principal part of the repeat in a polymer.
- Keep number of figures under control. If the info in two can be depicted by one, it is better to omit one of them.

Things to check for

- Run CIF through publCIF to check references.
- Run CIF through Platon to…
  - Do validation, as some Platon tests not in checkCIF, particularly FoFc tests for twinning, mismatch of files, completeness, unrefined Flack parameter. This needs the CIF and FoFc (hkl) files to be present. If a multi-structure CIF, the hkl files need to be concatenated.
  - If any doubts, run a test refinement (use Platon CIF2SHELXL button to prepare files) – won't work for twins or highly restrained structures.
  - Platon 'calc all' can be used to check parameters reported in text. Frequently there are errors or missing s.u.s, or incorrect symmetry codes.

Using Platon

- CIF2SHELXL button to generate ready-to-go .ins and .hkl files for quick SHELXL run.
- Should get essentially same result as author.
- Some authors use DAMP 0 0 which gives s.u.s but zero shifts, even for an unconverged model - beware!
- Compare the ORTEP view from this refinement with the published one - can reveal manipulation of Uij in CIF or plot.

Requesting revisions

- Pass referee reports and your own comments to authors.
- Try to be helpful, even if rejecting.
- No referee identifying tags in any attachments, e.g Word or PDF. Ideally, use text only files.
- Instruct authors clearly what to do to revise and upload files - web links in the on-line template letters (you can request these templates to be customised).
- Set a time limit (1 month max). For 2nd revisions, use a shorter time limit. We are trying to keep to an average publication time for papers of < 1 month.
- Ask that the report be returned annotated with author explanations of action applied to each point.

Handling the revised paper

- Check (changed) things again.
- New refinements require new structure factors.
- If OK, move to acceptance.
- If not OK, request further revisions or reject.
- Some authors won't or can't do more than superficial changes, even if you see great potential for writing a nice story.
- It is easy to get trapped with a paper, where you offer the possibility of acceptance if the authors can just write something better, but then you find the authors are not able to manage and you end up doing a lot yourself or having to reject. Thus, if the paper looks far too poor at the beginning, it may be better to reject and indicate what is needed. Sometimes you get almost the same thing back next day as a new submission! After two attempts to submit a revised version of a rejected paper, you can tell the authors the paper will not be considered again (at your discretion). If they persist, you an ask Chester to permanently reject a paper.

Editing final CIF

- Make any changes you deem necessary to the CIF then upload final version through review system.
- Considerable editorial changes and corrections allowed. When the language is poor, it is up to you how generous you want to be with rewriting a paper. Can consume time. Most authors grateful for help, but they have to learn they may need to seek local help or services. We are not obliged to rewrite. If it is too bad, reject.
- The exptl_refinement text is often sparse with information, or has some standard text that bears little resemblance to reality. Check and update.
- In H-bond table, the calculated angles should be rounded to integers.
- We request authors to include their final .res files (or equivalent) in the CIF. Often they do not and you have to ask for this. It helps with reviews, especially when restraints are used, but not documented. Currently it is not obligatory if authors object.
- When accepting, you can have a standard or customised letter sent to authors.
- Notes to Chester only needed if there is something you need to draw their attention to when making up the proofs.