

Information for (New) Co-editors

This presentation was originally developed by Tony Linden and delivered at the induction for new co-editors held during the IUCr Osaka Congress in August 2008. It was rather quickly thrown together, but the contents may be useful as a general guide to co-editorial procedures. Tony last updated it in December, 2010.

For the co-editor induction at the IUCr Congress in Madrid, it has been updated slightly by Sandy Blake.

Topics

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- Selecting referees
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Notes for Authors (NfA)

- Please make yourself thoroughly familiar with the current Notes for Authors.
- Authors are required to adhere to the NfA, but often do not read them.
- Be familiar with journal style requirements, *e.g.*, atom labels do not have parentheses, whether they occur in Figures, Tables or running text.
- Read through the handbooks and other information supplied, *e.g.*, the ‘useful links’ section of your co-editor home page.

Initial assessment of paper

Try to do this as quickly as possible (to referee within 24 - 48 h)

- If the structure is clearly wrong, the CIF is deficient, or ...
- the Abstract and Comment are far too short and/or totally incomprehensible ...
- **Don't waste time on it. There is no need to use a referee at this stage.**
- **Write a short, polite note to say paper rejected. Give some of the reasons.**
- Acta E style papers are sometimes submitted to Acta C. Reject and say the format looks more appropriate for Acta 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 the previous co-editor to ask why the paper was rejected.
- Duplicated structures need to have very substantial reasons to be published again (*e.g.*, much improved model or significant extension of earlier discussion - see Notes for Authors). [Acta E story]

Selecting referees and time frame

- Use at least one referee initially: different people spot different things.
- People who (a) are knowledgeable in the field, (b) know the *Acta* requirements, (c) are fair, and (d) who respond quickly, are best.
- If other results or chemistry reported, you may need a specialist in that area.
- Reports should ideally come back within one week. If a 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 has passed, enquire if action can be expected soon, rather than waiting for authors to respond.
- 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!

The roles of Co-editor and Section Editor

- Co-editor has full freedom to handle the paper as he or she chooses, right up to the fully acceptable product.
- Section Editor (or Deputy) 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 involve the co-editor unless the whole paper needs serious work.
- Messages to Sean get sent automatically to the handling co-editor. This is meant as a learning aid so you can see if you have missed something. If anything is unclear, ask. It is also 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 raise this with the authors, but advise the Section Editor. Some (inexperienced) authors do strange 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 intramolecular C-H \cdots X H-bonds (*e.g.*, C-H and X-C are parallel).

Things to check for

- Check that symmetry codes are present (and correct!) in text for all symmetry-related atoms discussed, *e.g.*, of contacts, H-bonds.
- Also in Figure captions and Tables.
- 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 diagrams, the labels without symmetry codes must correspond to the position of these atoms defined by the model.
- In packing diagrams, the cell axes must be shown and labelled. Omit H atoms not involved in contacts. Ball-and-stick style is usually clearer than ellipsoids.
- 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 information 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 full validation, as some PLATON tests are not in checkCIF. This needs the CIF and fcf (hkl) files to be present. If a multi-structure CIF, the hkl files need to be concatenated.
 - Run a test refinement (use PLATON CIF2SHELXL button to prepare files). If major parameter shifts or changes in R/wR/S appear, there is something wrong. This test won't work for twins or highly restrained structures.
 - We also request that authors include their final .RES file (or equivalent) in the CIF. Often they do not and you have to ask for this. It can be used for a test refinement and helps with reviews, especially when restraints are used but not documented, sometimes the .RES doesn't match the CIF at all. Currently .RES files are not compulsory, but so far authors have always supplied this when asked. Should they be compulsory?
 - PLATON 'CALC ALL' can be used to check parameters reported in text: the output .LIS file contains almost all imaginable parameters! Frequently there are errors, 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!
- ! Recent example: the number of refined parameters much less than expected – authors had used EADP for a slew of atoms on different sites.
- 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.
- ! Be alert for any tags which might identify a referee in any attachments, *e.g.*, Word or PDF documents. Ideally, use text-only files.
- Instruct authors clearly what to do to revise and upload files – see the web links in the on-line template letters (you can request these templates to be customised).
- Set a time limit (1 month max). For second cycle of revisions, use a shorter time limit. We are trying to keep to an average publication time for papers of < 1 month.
- Ask that the referee 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 and Figures.
- 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 can ask Chester to permanently reject a paper: any attempt to re-submit is then automatically blocked by the submission system if it recognises the paper.

Editing the final CIF

- Make any changes you deem necessary to the CIF then upload the final version through the review system.
- Considerable editorial changes and corrections are allowed: if it is easier to fix things yourself than to get the authors to do them that is OK. When the language is poor, it is up to you how generous you want to be with rewriting a paper. This can consume a lot of time. Most authors are grateful for the 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 paper.
- 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.
- When accepting, you can have a standard or customised letter sent to authors.
- Notes to Chester are only needed if there is something you need to draw their attention to when making up the proofs.

Some final comments

You are not alone:

If you can't find some piece of information, or you are having problems with a borderline decision, you can contact Tony (or Sandy) for advice. Send a succinct explanation of the problem and attach any relevant files.

Many eyes make a better paper:

Referees, co-editor, Section Editor, Sean.

Be suspicious:

Some authors make mistakes you never would.

References:

Check that references do what the authors claim.

- Start of Comment: introductory references ... "catalytic studies"?
- Structure comparison: "My bond length is shorter than my neighbour's" – insist on a comparison with the full literature.

Some final comments

You can get time off:

If you are going on holiday, have other obligations for a while, or feel you have a backlog of Acta papers, simply ask Sean to set your quota lower (or even to zero) for a while, or ask him to make you inactive for a period.

Note: Co-editors with a quota of zero receive resubmissions of papers they previously rejected, while those who are inactive do not.

Current JComm Notes for Section E co-editors:

Some of the tips there are also highly useful for handling Acta C papers.

And finally a message from Tony:

“Please emphasise that that it is important to be courteous and respectful in communications, no matter how stubborn, stupid, pig-headed, or frustrating an author may appear to be. Some authors claim to have attended to all of the long list of points you might have given them, but the revised version has changed almost imperceptibly and this can lead you to the point of exploding. Take a deep breath before writing back.”