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. This is an informal document, but the contents may be useful as a general guide to co-editorial procedures. Tony last updated it in October, 2014, and Paul has made some additional small changes in 2017.

Topics

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- Selecting referees
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- The roles of Co-editor and Main Editor
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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.
- We accept submissions for which the text of the paper is a Word document and the CIF only contains the technical data. Beware that the review PDF file sometimes looks a little odd when Word is used, so not necessarily the authors' fault.

Acta C, or E, or…?

- Be familiar with the current Notes for Authors for Acta E as well. E has changed format several times and might start to look more like C has been in the past.
- Look at the C editorials (Jan 2015, Jan 2017) to see how we are trying to shift the focus and style of papers. Look also at recent issues of C to see the style of paper we would like to encourage. We are strongly encouraging the inclusion of more chemistry in the papers and like them to tell a story.
- However, the new style has not been accepted fully and we still get our traditional papers, so these have to be tolerated as long as the results and discussion are substantial.
- It is often hard to decide if a short paper is really C material or should be for E. Look at papers in recent issues to get a gauge for suitable length. If in doubt and you think it is an E paper, reject and advise the authors to submit to E.
- Papers that just report the standard metrics of a structure using mostly the data already in the CIF are better in E. Some extended discussion is needed that goes beyond the basic CIF information and, ideally, contains some other scientific results and discussion thereof. Some people use a yardstick that the discussion should make at least 6 points that are not derivable directly from the CIF info.

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.
- ℹ Rejected papers, if resubmitted, usually automatically come back to same co-editor.
- ℹ 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 or Sean Conway will be able to supply you with previous emails.
- ℹ 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).

Selecting referees and time frame

- Use at least one referee: 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. Or they find all the typos, ignore the science. **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 Main Editor

- Co-editor has full freedom to handle the paper as he or she chooses, right up to the fully acceptable product.
- How much editorial help you give an author to improve poor writing is up to you.
- One of the Main Editors will read the proofs:
- Hopes nothing further needed. Might 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. If there are significant issues, either chemical or crystallographic, we may ask the co-editor to check through again and make further corrections/suggestions.
- Messages about proofs to Sean from the Section Editors get copied automatically to the handling co-editor. No action is required. This is meant as an informational 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 one of the Main Editors.

! 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, unless these are integrally related to the chemical problem that the paper addresses.
- Results and discussion
  - 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···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 (usually already done in Chester).
  - Run a test refinement (use PLATON CIF2SHELXL button to prepare files if SHELXL-97 was used by the authors, shredcif with a SHELXL-2014 CIF). 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 unless the CIF is a SHELXL-2014 one.
  - 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.
  - PLATON 'CALC ALL' can be used to check many 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 in papers.
  - We very strongly encourage use of SHELXL-2014 over -97 (if the authors use SHELXL). You can ask the authors to justify why they have not used SHELXL-2014, and ask them to re-refine if they don't have a good reason.

Using PLATON

- CIF2SHELXL button (or SHREDCIF) 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.
- 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. It is hard to see what was changed if they upload a new version of the paper and do not tell you what they did/did not do.

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/WORD file

- Make any changes you deem necessary to the CIF/WORD file 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.
- Check that **references** report what the authors claim and are relevant, particularly in the introduction. Use *publCIF* to verify all references in the text are in the ref. list & v.v.
- Introduction: introductory references should be relevant.
- Structure comparison: “My bond length is shorter than that in a related compound.” insist on a comparison with the full literature and that they tell you what that cited compound actually is.

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 Paul Raithby, Larry Falvello or Jonathan White for advice. Send a succinct explanation of the problem and attach any relevant files.

Many eyes make a better paper:
Referees, co-editor, Main Editor, Sean.

Be wary:
Some authors make mistakes you never would.

Manage your time:
We understand you are all busy with many things and sometimes priorities have to be set. It is important for the journal that you do not let editorial work fall behind. If you have other obligations for a period, it is better to tell us sooner than let a paper get 3 or more months old, especially if it is sitting on your desk waiting for action by you. We can reassign papers if necessary. Think of it from your perspective as an author. When you submit a paper yourself to any journal, you expect an answer within a reasonable time, so our authors expect the same from you. Ideally, try not to let a paper sit on your desk for more than a couple of days at each point where action by you is the next step.

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 Notes for Section E authors:
Some of the requirements there are also highly useful for handling Acta C papers.

And finally:
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. Most authors are usually very grateful for any assistance you give and mostly do not object when you tweak their text.

We are always very grateful for your voluntary work on behalf of the journal and for all of your efforts as a co-editor. We hope you enjoy your time on the editorial board.