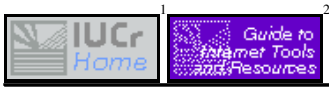

IUCr Journals – Submission and Consultation

Traditionally, publication of research results in journals has been effected through the skills of trained technical editors and typesetters, and specialized publishing houses have controlled the complex processes of setting type, composing and printing. The widespread availability of modern desktop publishing packages has encouraged authors to believe that they can partake in the technicalities of publishing their work. However, there is a danger that they may become seduced by the artistic potential of their software, and lose sight of the greatest strength of electronic publishing, which is to store information in a structured and usefully retrievable form. The IUCr encourages authors to submit their work in a **structured** fashion, to take best advantage of this strength.

CIF Submission to Structural Journals

The Crystallographic Information File[3](CIF) is a simple file format ideally tailored to the requirements of crystallographic data storage and exchange. One of the IUCr's journals, *Acta Crystallographica Section C – Crystal Structure Communications*[4], **only** accepts submissions in CIF format. Other journals reporting structural results, such as *Acta Crystallographica Section B – Structural Science*[5], also make use of CIF submissions.

Acta Crystallographica Section C

A typical protocol for an author wishing to report a structure determination to *Acta C* is as follows.

1. Perform an experiment, solve and refine the structure of a compound.
2. Write the experimental results to a CIF output file. This is achieved in many cases as a standard output option of the solution or refinement software employed. For example, the following packages include CIF output subroutines:
   - *NRCVAX*[6]– an integrated system with user–friendly interface
   - *SHELXL93*[7]– a structure refinement program
   - *Xtal*[8]– an integrated system of crystallographic solution, refinement and graphics programs

   Alternatively, a utility program may be used to translate results from a different format to CIF. Examples of such software include:
   - *PARSTCIF*[9]– for converting output from the molecular geometry analysis program *PARST* to CIF format
   - *PLATON*[10]– geometry analysis, graphics and validation checks

   In extremis, it is possible (if tedious) to construct a CIF by hand or by writing your own software utility.
3. Mail a copy of the complete CIF to **checkcif@iucr.ac.uk** to receive an automatically–generated check report on the syntactic validity of the file and the result of some checks of the self–consistency and integrity of the reported structure.
4. Add the discursive text of the paper as additional text fields to the CIF.
5. Mail the result to **printcif@iucr.ac.uk** to receive a PostScript file displaying the formatted version of the paper that will be seen by editors and referees.
6. Make any changes necessary to the prospective submission as a result of the reports generated by **checkcif** and **printcif** and ensure that the submission conforms to the instructions in **Notes for Authors**.[11]

[1] http://www.iucr.ac.uk/iucr–top/welcome.html
[2] int.index.html
[3] http://www.iucr.ac.uk/cif/home.html
[4] http://www.iucr.ac.uk/journals/acta/actac.html
[5] http://www.iucr.ac.uk/journals/acta/actab.html
[6] http://laue.chem.ncsu.edu/refs/nrcvax.html
[7] http://www.lmcp.jussieu.fr/sincris/logiciel/prg–shelxl.html
[8] http://www.crystal.uwa.edu.au/xtal/
[9] http://www.lmcp.jussieu.fr/sincris/logiciel/prg–parst95.html
[10] http://www.lmcp.jussieu.fr/sincris/logiciel/prg–spek.html
[11] http://www.iucr.ac.uk/journals/acta/actac_notes.html

7. E–mail the submission to **med@iucr.ac.uk**. Include your covering letter as a text field **within** the CIF.
8. Upon receipt of an acknowledgement and manuscript handling code, transfer structure factors and PostScript or HPGL graphics to the *incoming* directory of the anonymous FTP host[12] **ftp.iucr.ac.uk**.
9. Send an e–mail to **med@iucr.ac.uk** indicating which files you have transferred.
10. Fax or post by ordinary mail a copy of the Transfer of Copyright form.[13]

More details are supplied in **Notes for Authors**,[14] and in the booklet *A Guide to CIF for Authors*, available by post from IUCr, 5 Abbey Square, Chester CH1 2HU, England, or as an electronic file[15] in Adobe PDF format.

Other structural papers

At the time of writing, submissions to *Acta B* may include CIF components. A more coherent policy for submitting structural papers to *Acta B* (and, ultimately, to *Acta D*) is under development. Latest information is always carried in **Notes for Authors**.[16]

Electronic Submission of Other Papers

As mentioned above, the full benefits of electronic submission are only realized when the papers submitted conform to a detailed structural model. For this reason, we are developing a description of the contents of the journals in SGML (the Standard Generalized Markup Language convention accepted by the International Standards Organization). When this is complete, template files will be distributed to authors to permit the most efficient use of word–processor packages such as Microsoft Word and WordPerfect, or the technical typesetting macro package LaTeX.

Full details of these initiatives will be posted on the IUCr web pages[17] as they are developed.

Meanwhile, electronic submissions in

- Wordperfect, versions 4–6
- Microsoft Word for Macintosh, versions 4, 5, 6 and onwards
- Microsoft Word for Windows, versions 6 onwards
- plain TeX
- standard LaTeX 2.09 and LaTeX 2epsilon packages

are welcomed, but without a guarantee that they will be used directly.

Graphics files in PostScript or HPGL formats are also welcomed.

Full details of submission policy and practice are always available through **Notes for Authors** on the journals' home pages.[18]

Consultation of IUCr Journals Online

The contents pages of recent and current issues of the journals may be browsed online through the IUCr web pages.[19]

Available are

- Cover artwork
- Paper reference
- Paper title
- Authors' names
- Synopsis of paper

[12] http://www.lmcp.jussieu.fr/~epelboin/conf/ftp/ftp–gen.html#anonymous
[13] http://www.iucr.ac.uk/journals/copy96.pdf
[14] http://www.iucr.ac.uk/journals/acta/actac_notes.html
[15] http://www.iucr.ac.uk/journals/acta/cifguide.pdf
[16] http://www.iucr.ac.uk/journals/acta/actab_notes.html
[17] http://www.iucr.ac.uk/welcome.html
[18] http://www.iucr.ac.uk/journals/index.html
[19] http://www.iucr.ac.uk/journals/index.html

and, for *Acta Crystallographica Section C*, also

- Chemical formulae
- Structural schemes
- Authors' addresses
- Received/accepted dates
- The full set of reported structural data in CIF format

Authors may also interrogate the journals production database for details of the status of their submitted paper.[20]

Studies are in hand to make available the full text of abstracts and papers to subscribers in the near future.

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[20] http://www.iucr.ac.uk/journals/status.html
[21] int.index.html
[22] http://www.iucr.ac.uk/.html/bm.html