Chemical Communications

Instructions for Authors (2004)

Also see: www.rsc.org/illustrations and www.rsc.org/electronicfiles

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1 Refereeing policy

Chemical Communications publishes preliminary accounts of original and significant research that will appeal to a wide general readership or be of exceptional interest to the specialist. Following publication of a communication a full paper should be prepared and submitted to an appropriate journal. Acceptance in *Chemical Communications* does not guarantee subsequent publication in the RSC's journals. No work submitted to *Chemical Communications* should simultaneously be submitted to or be under current consideration by any other journal.

Contributions which have appeared or have been accepted for publication with essentially the same content in another journal are not suitable for consideration by *Chemical Communications*. In addition the unnecessary fragmentation of results to maximise the number of publications is unacceptable. Unnecessary fragmentation is itself a valid reason for rejection of manuscripts.

Authors must also include a brief statement justifying why their paper should be published in *Chemical Communications*.

Each communication deemed suitable for consideration as a submission will be assessed by at least two independent referees. Authors are invited to suggest suitable referees for their communication. However, it would not normally be appropriate to use only those referees nominated by the author. The decision to accept or reject a paper will be made on the basis of two agreeing reports. Authors who disagree strongly with the result may appeal to the *Chemical Communications* Editorial Board through the Managing Editor at Cambridge.

It is the author's responsibility to declare and cite all unpublished work directly related to any new submission to *Chemical Communications*, including work in press or submitted to another journal.

Short articles that are detailed enough should be submitted as a complete account to the appropriate RSC journal.

2 Administration

Manuscripts should be directed to the appropriate Editor (see inside front cover or www.rsc.org/is/journals/current/chemcomm/cccasse.htm for details), who will acknowledge receipt, but authors should contact the Cambridge office if they have not had a response after a reasonable time. All authors submitting work for publication are required to sign an exclusive Licence to Publish, without which publication cannot proceed. The Licence to Publish should be agreed during the online submission process (http://www.rsc.org/submissions). Alternatively a completed form can be sent to the Editor by fax or post. (The form can be obtained from www.rsc.org/is/journals/current/coplic.htm)

Authors must provide, in addition to their full contact address, telephone and fax numbers and an E-mail address. They should state explicitly if fax and/or E-mail should not be used to send referees' comments.

Communications will be refereed as quickly as possible and a decision will be sent to the author when two concurring opinions are received.

Proofs will be sent to the person submitting the article or to a person designated by them.

3 Preparation of manuscripts

3.1 General

Communications should be brief and may not exceed two pages in the printed form including tables and illustrations. Authors

are encouraged to use the template, available at www.rsc.org/is/journals/templates/templates.htm for preparing their submissions.

Lengthy introductions and discussion, extensive data, and excessive experimental details and conjecture should not be included. Figures and tables will only be published if they are essential to understanding the paper.

The experimental evidence necessary to support a communication should be supplied for the referees and eventual publication as *electronic supplementary information*.

In certain circumstances where additional space is required to present the chemistry clearly to the community a third page may be allowed.

Authors wishing to submit a three page communication **must**:

- Provide a statement giving the reasons why the work requires an additional page. (In addition to the *statement* requested below)
- Submit the work electronically using the RSC's manuscript template (see www.rsc.org/is/journals/templates/templates.htm)

A request for a third page may only be made on submission. Requests for an additional page will not be considered after this stage. Comment on the suitability of an additional page will be sought from the referees however any final decision will be made by the Editorial Office.

Statement – A note giving the reasons why the work should be published in *Chemical Communications* should be provided. When preparing the statement the following criteria should be addressed:

1. The significance and novelty of the work should be highlighted
2. Interest to either the wide general readership or exceptional interest to the specialist should be highlighted

Referees – A few suitable referees may be suggested: please give full names, E-mail addresses and affiliations.

Copy – The first page must include the following information:

- A succinct title indicating the content and serving as a point of entry for information retrieval purposes, with the first word only capitalised.
- The authors' names, with one forename for each, with an asterisk indicating the author for correspondence.
- The establishment(s) at which the work was carried out and each author's affiliation.
- A **one**-sentence summary stating the main finding(s).

Patents – All patents relating to work contained in a new submission must be filed before submission of an article.

Graphical abstract – **All** communications should include a graphical abstract. Maximum size 40 × 95 mm, for the contents list. Examples of style and format may be found in any recent issue. This should also include a brief (~30 word) summary of the novel aspects of the work for publication in the Contents List, and the graphic may be in colour.

References and notes – References are cited in the text using superior numbers and typed in numerical sequence in the following style: A. N. Author, *Chem. Commun.*, 1998, 1–3. Where possible a page range is preferred, however either format is acceptable. A list of standard journal abbreviations in available on our web pages (www.rsc.org/is/journals/authrefs/jabbr.htm). Authors are encouraged to check our Reviews website (http://www.rsc.org/reviews) to ensure that they have cited relevant recent reviews.

Illustrations – Structure reference numbers must be cited in numerical order in displayed formulae. Detailed guidelines on the preparation of illustrations can be found at www.rsc.org/authors

Colour – Colour may be used free of charge where scientifically necessary. Full guidelines on the use of colour are available at http://www.rsc.org/authors

3.2 Submission of articles

Authors are encouraged to send submissions to the Journal in electronic form using the RSC e-submission service.

3.2.1 Online submission of Articles [E-submissions]. Online submission web page: www.rsc.org/submissions

Articles should be submitted as a single file in either MS Word or PDF format. This PDF facilitates online refereeing and allows manuscripts to be handled more accurately and efficiently by the Editorial Offices. Please note that when an article is accepted for publication, a MS Word (or similar native format) version of the manuscript and separate copies of the *artwork* in TIFF, EPS or PDF formats at 600 dpi will be required at that time for proof preparation. It would be helpful if PDF graphics were produced using the "PDF Creation Files" job options from our web site: www.rsc.org/is/journals/templates/templates.htm. Unfortunately PDF text files are **not** suitable for proof preparation.

Further information on which type of electronic files are suitable for submission may be found at www.rsc.org/electronicfiles

The RSC e-submission service allows any number of files to be uploaded to either the Cambridge Editorial Office or US Associate Editor Offices. The following files and information should be provided:

a. The manuscript as a single file (containing text and figures) in either PDF or MS Word format.
b. Crystallographic data in CIF format (if appropriate, see Section 5)
c. Data for deposition with the ESI service, including any experimental evidence necessary to support the communication
d. Details of any relevant articles in press or 'submitted to' references (please give reference or include PDF file)
e. A graphical abstract for the contents page
f. Names of potential referees
g. A justification of why the work merits urgent publication in *ChemComm*.

After e-submission your file will be acknowledged by the Editorial Office as soon as possible. Authors should contact the Editorial Office if they have not received an acknowledgement within 4 working days. Authors should not forward more than one version of their manuscript or submit the manuscript by post or E-mail to avoid errors in manuscript handling by the Editorial Office.

For manuscripts submitted online a printed copy of the manuscript will **not** be required.

3.2.2 Postal Submission of Articles. For postal submissions all of the electronic files should be supplied on a disk or CD-ROM. Crystallographic material for the referees and/or deposition must also be supplied where applicable (see section 5). Copies of any related, in press articles or articles submitted to another journal for consideration should also be provided.

3.2.3 Requirements for revised articles and material for proof preparation. Revised manuscripts should preferably be sent to the Editorial Office by electronic file upload (**www.rsc.org/submissions**). Alternatively files may be forwarded by E-mail to chemcomm@rsc.org or by post. Revised manuscripts sent by post can be accepted on 3.5 inch disk, ZIP disk or CD-ROM and should be accompanied by a printed copy of the manuscript. Please ensure that the electronic version is identical to the hardcopy.

The revised files should be sent in the formats given in the separate Guidelines on submitting files for proof preparation www.rsc.org/pdf/authrefs/proofprep.pdf

Additional information on acceptable file formats for submission of a revised manuscript may be found at www.rsc.org/electronicfiles

4 Electronic Supplementary Information (ESI) service

Authors are encouraged to deposit bulk information (such as primary kinetic data, spectra, programs, etc.) with the RSC's ESI service. Any experimental evidence necessary to support a communication must be supplied. Such data will be made freely available online if the manuscript is accepted for publication. The electronic data should be supplied in one of the formats below (other formats may also be acceptable)

- Word
- WordPerfect
- JPEG/GIF (max 640 × 480 pixels)
- MOL (or PDB)
- Crystallographic Information File (CIF)

For postal submissions the electronic files should be supplied on disk. Further details: www.rsc.org/esi

5 Publication of X-ray crystallographic work

Crystallographic work will be assessed in the context of the chemistry being presented and should normally be fully refined. Where refinement is incomplete, or the structure displays any unusual features or other problems, the authors should provide suitable details to show that publication of the structure determination is appropriate.

Authors wishing to submit X-ray crystallographic work are strongly encouraged to consult the full guidelines before submitting such work (available at www.rsc.org/is/journals/authrefs/cryst.htm, or on request from the Editorial Office).

Brief details of the data collection and structure analysis should be given in a footnote or in the Notes and References section. The following information should be given in the manuscript:

1. Chemical formula and formula weight (M)
2. Crystal system
3. Unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, temperature
4. Space group symbol (if non-standard setting give related standard setting)
5. No. of formula units in unit cell (Z)
6. Linear absorption coefficient (μ)
7. Number of reflections measured and/or number of independent reflections and R_{int}
8. Final R values (and whether quoted for all or observed data)

The following example demonstrates the application of the recommendations:

Crystal data: $C_{28}H_{31}BrCl_4N_2O_{14}Pd$, M = 947.66, orthorhombic, a = 11.0969(14), b = 17.197(2), c = 19.604(3) Å, U = 3741.0(9) Å^3, T = 173 K, space group $P2_12_12_1$ (no. 19), Z = 4, μ(Mo-Kα) = 1.9 mm^{-1}, 6013 reflections measured, 5665 unique (R_{int} = 0.031) which were used in all calculations. The final $wR(F^2)$ was 0.099 (all data).

Selected bond lengths and angles, with estimated standard deviations, should normally be included in the figure captions and be restricted to significant dimensions only. Authors should also submit all supplementary crystallographic data as a Crystallographic Information File (CIF) file electronically to the editor to whom the manuscript has been submitted. This should include: a table of final fractional atomic coordinates; any calculated coordinates (*e.g.* hydrogen); a full list of bond lengths and angles with estimated standard deviations; a full list of displacement parameters in the form B_{ij} or U_{ij} (in Å^2 or pm^2); FULL details of the solution and refinement.

Supplementary crystallographic data will be passed to the Cambridge Crystallographic Data Centre (CCDC) as part of the assessment process. Each structure will be assigned a separate CCDC number which will be detailed in the subsequent crystallographic report. Data will be held in their confidential archive until publication of the article, when they will be entered into the Cambridge Structural Database (if an organic carbon is present) while purely inorganic data will be forwarded to the Fachinformationszentrum Karlsruhe. Enquiries for data can be directed to CCDC, 12 Union Road, Cambridge, UK CB2 1EZ, deposit@ccdc.cam.ac.uk, Fax +44 (0) 1223 336033

If the article is not published by the RSC, these data will remain in the CCDC's confidential archive. If the crystal structure(s) are then published elsewhere, the CCDC Deposition Number(s) detailed in the crystallographic report should be quoted in that publication and the CCDC advised of the new journal and the appropriate reference.

The Cambridge Crystallographic Data Centre (CCDC) have a freely available programme which allows users to add RSC required information to cif files *via* a user-friendly graphical interface. Download EnCIFer for free at http://www.ccdc.cam.ac.uk/prods/encifer

The IUCR also have a free cif checking facility available at http://checkcif.iucr.org Authors are encouraged to validate their cif files before submission.

5.1 Publication of Powder Diffraction Studies

5.1.1 Unrefined Powder Diffraction Data. Powder diffraction data should normally only be given where the data forms a part of the discussion presented in the paper and should be restricted to new materials. In such cases, the following experimental details should be provided as part of a footnote or reference:

1. Diffractometer name and model
2. Radiation wavelength
3. Temperature of data collection
4. 2θ collection range
5. Unit cell dimensions, if determined

Tables of 2θ data, or diagrams showing diffraction patterns of reaction products, should not normally be published in print, unless they have some distinct feature of relevance that requires such material to be present. In all other cases, such data may be provided as supplementary material, simultaneously with the paper, for deposition with the RSC's Supplementary Publications scheme.

For cases where the materials are new but have similar powder data to other, well characterised, materials, such data should not usually be included in the paper.

5.1.2 Refined Powder Diffraction Data (Where Atomic Coordinates Have Been Determined). Details of the data collection and structure analysis should be given in a footnote or in the References/Notes section. The following information should be given:

1. Diffractometer name and model
2. Radiation wavelength
3. Temperature of data collection
4. 2θ collection range
5. Step size
6. Chemical formula
7. Formula weight
8. Unit cell dimensions
9. Space group
10. Z

11. Number of reflections
12. Final R values (R_{wp}, R_{exp} and R_I) and method of background treatment

A table of *atomic coordinates* may be provided if it forms an important aspect of the study. Selected bond lengths and angles, with estimated standard deviations, should be included in the figure captions and be restricted to significant dimensions only.

For Rietveld refinements, an observed + calculated + difference profile plot may be given for each structure determination, except where a significant number of similar refinements have been carried out. In such cases, only the minimum number of representative plots should be included in the article, with additional plots being provided as supplementary material.

A perspective plot (or similar) of the structure should normally be provided. This should be produced in the same style as that detailed for illustrations of single crystal structure determinations.

Authors should submit the following supplementary data for use by the referees. This should be provided electronically, or if no electronic version is available, as two hard copies at the time of submission.

1. A table of final fractional atomic coordinates
2. Any calculated coordinates (*e.g.* hydrogen)
3. A full list of bond lengths and angles with estimated standard deviations
4. A full list of displacement parameters in the form B_{ij} or U_{ij} (in Å^2 or pm^2)
5. Details of the refinement (as given above in points 1–12)
6. Profile difference plots for all analyses

Supplementary powder diffraction data (where atomic coordinates have been determined) will be deposited by the RSC with the Cambridge Crystallographic Data Centre (CCDC) as part of the assessment process. Each organic or metallo-organic structure will be assigned a separate CCDC number. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and metallo-organic compounds will be entered into the Cambridge Structural Database. Post-publication requests for individual data sets should be directed to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, deposit@ccdc.cam.ac.uk, fax +44 (0)1223 336033.

If the article is not published by the RSC, supplementary crystallographic data will remain in the CCDC's confidential archive. If the crystal structure(s) are subsequently published elsewhere, the CCDC should be advised of the new journal and the appropriate reference.

5.2 Guidelines for macromolecular X-ray and NMR structures and sequence data

Novel macromolecular structures

All manuscripts that report novel macromolecular three-dimensional structures at the level of individual atomic positions must be accompanied by deposition of the required structural data in the appropriate database (usually PDB or NDB – see contact details below) to support the conclusions drawn. For X-ray structures, atomic coordinates and structure factor data are required. For NMR structures, data should include all resonance assignments and restraints used in structure determination (NOEs, spin-spin coupling constants, amide exchange rates, etc.) as well as atomic coordinates derived for both an individual/average structure and an acceptable family of structures.

Sufficient information must be supplied to satisfy referees of the validity of the conclusions drawn. For X-ray structures, PDB header information (*i.e.* Rmerge, completeness, multiplicity and I/sigmaI (both overall and in the outer resolution shell) for data, and Rcryst, Rfree and the bond and angle deviations for coordinates), a Ramachandran plot and preferably real space R-factor must be supplied. For NMR structures equivalent data (number of restraints (NOEs and *J*-couplings), RMS restraint deviation etc.) plus resonance assignments in the case of NMR structures must be supplied. All the above data should be included in as summary data tables in the manuscript, or as ESI.

Deposited files must be released immediately on publication. A six-month delay will be considered only in exceptional circumstances. Articles will not be published until the relevant PDB or NDB accession number has been provided. These codes should be quoted both in the experimental section of the manuscript and in the abstract (or article header information) so that abstracting services will access them.

Sequence data

Newly reported nucleic acid or protein sequences must be deposited with the appropriate database: EMBL, GenBank, DDBJ, SWISS-PROT or PSD (see below for contact details). Deposited files must be released immediately on publication of the article, which will not be published until an accession number is quoted in the experimental section of the manuscript and the abstract.

Contact details for structure and sequence databases

Protein Data Bank, pdb.rutgers.edu, deposit@rcsb.rutgers.edu or www.ebi.ac.uk/msd/, pdbhelp@ebi.ac.uk

Nucleic Acids Database, ndbserver.rutgers.edu, ndbadmin@ndbserver.rutgers.edu

EMBL Nucleotide Sequence Submissions, www.ebi.ac.uk/Submissions/, datasubs@ebi.ac.uk

National Center for Biotechnology Information (GenBank), http://www.ncbi.nlm.nih.gov/, info@ncbi.nlm.nih.gov

DNA Data Bank of Japan, http://www.ddbj.nig.ac.jp/, ddbj@ddbj.nig.ac.jp

SWISS-PROT submissions, http://www.ebi.ac.uk/, datasubs@ebi.ac.uk

Protein Information Resource (Protein Sequence Database, PSD), www-nbrf.georgetown.edu/pir/, pirmail@nbrf.georgetown.edu

6 Animal Welfare

In cases where an experiment involves the use of live animal, the Methods section of the manuscript should include a statement that all experiments were performed in compliance with the relevant laws and institutional guidelines, and should identify the institutional committees that have approved the experiments where applicable. Referees may be asked to comment specifically on any cases in which concerns may arise.

7 Characterisation within Chemical Biology and Medicinal Chemistry

Where compounds are synthesised for testing in biological systems, sufficient evidence for purity and identity must be provided such that the results of the experiment may be trusted.

The homogeneity of oligomeric compounds (peptides, saccharides, nucleotides etc.) should be determined by HPLC analyses or by other appropriate analytical methods (*e.g.* capillary electrophoresis) with a purity of not less than 95%.

8 Submission checklist

- A copy of the communication as specified in section 3
- A justification of why the work merits urgent publication in *Chemical Communications*.

- Full contact address, telephone and fax numbers and an E-mail address.
- Suggested referees – please give full names and affiliations.
- A graphical abstract for the contents page, including a short statement of novelty
- Copies of any references submitted to or in press with any other journal
- Completed Licence to Publish.
- Crystallographic data (if applicable) in CIF format.
- Supplementary information for the referees if appropriate, and data for deposition with the ESI service, including the experimental evidence necessary to support the communication
- Identifying data for any microorganisms described.

Further information can be obtained from **Dr Sarah Thomas**, *Chemical Communications*, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 0WF, UK, tel +44 (0) 1223 420066, fax +44 (0)1223 420247, chemcomm@rsc.org