

Chemical Communications

Guidelines for Authors†

Also see: www.rsc.org/authorguidelines

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It is the author's responsibility to declare and cite all unpublished work directly related to any new submission to *Chemical Communications*, including work in press or submitted to another journal.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

Further notes on RSC policy on the initial assessment of submissions, and details of criteria for publication, can be found on ReSource.‡

2.0 Article types

2.1 Communications

Communications should be brief and may not exceed three pages in the printed form including tables and illustrations. Authors must use the template, available from the RSC web site,‡ 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.

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:

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

3.0 Supporting Information

Experimental information must be provided to enable other researchers to reproduce accurately the work. The experimental details and the characterisation data should preferably be provided as Electronic Supplementary Information although on occasion it may be appropriate to include some or all of this within the body of the communication. This will depend on the nature of the research being reported.

† For more detailed information on this topic, including guidelines for article layout, preparation of illustrations, presentation of experimental data, and supplementary information deposition, as well as links to useful websites, templates and other software resources, and authoring tools, see: <http://www.rsc.org/authorguidelines>.

‡ See <http://www.rsc.org/resource>.

3.1 Characterisation of new compounds

It is the responsibility of authors to provide fully convincing evidence for the homogeneity, purity and identity of all compounds they claim as new. This evidence is required to establish that the properties and constants reported are those of the compound with the new structure claimed. Referees will assess, as a whole, the evidence presented in support of the claims made by the authors.

The requirements for characterisation criteria are detailed below.

3.1.1 Organic Compounds. Authors are required to provide unequivocal support for the purity and assigned structure of all compounds using a combination of the following characterization techniques:

- (i) *Analytical.* Elemental analysis (within $\pm 0.4\%$ of the calculated value) is required to confirm $\geq 95\%$ sample purity and corroborate isomeric purity. Authors are also encouraged to provide copies of $^1\text{H}/^{13}\text{C}$ -NMR spectra and/or GC/HPLC traces, however, if satisfactory elemental analysis cannot be obtained copies of these spectra and/or traces must be provided. For libraries of compounds, HPLC traces should be submitted as proof of purity. The determination of enantiomeric excess of nonracemic, chiral substances should be supported with either GC/HPLC traces with retention times for both enantiomers and separation conditions (*i.e.* chiral support, solvent and flow rate) or for Mosher Ester/Chiral Shift Reagent analysis, copies of the spectra.
- (ii) *Physical:* Important physical properties, for example, boiling or melting point, specific rotation, refractive index, *etc.*, including conditions and a comparison to the literature for known compounds should be provided. For crystalline compounds, the method used for recrystallization should also be documented (*i.e.* solvent *etc.*).
- (iii) *Spectroscopic:* Mass spectra and a complete numerical listing of $^1\text{H}/^{13}\text{C}$ -NMR peaks in support of the assigned structure, including relevant 2D NMR and related experiments (*i.e.* NOE, *etc.*) is required. As noted in (i), authors are encouraged to provide copies of these spectra. Infra Red spectra that support functional group modifications, including other diagnostic assignments should be included. High-resolution mass spectra are acceptable as proof of the molecular weight provided the purity of the sample has been accurately determined as outlined above.

The synthesis of all new compounds must be described in detail. Synthetic procedures must include the specific reagents, products and solvents and must give the amounts (g, mmol, for products: %) for all of them, as well as clearly stating how the percentage yields are calculated. They must include the ^1H , ^{13}C and MS data of this specific compound. For multistep synthesis papers: spectra of key compounds and of the final product should be included. For a series of related compounds at least one representative procedure which outlines a specific example that is described in the text or in a table and which is representative for the other cases must be provided.

3.1.2 Polymers. For all soluble polymers an estimation of molecular weight must be provided by a suitable method, *e.g.* size exclusion chromatography, including details of columns, eluents and calibration standards, intrinsic viscosity, MALDI TOF, *etc.* in addition to full NMR characterization (^1H , ^{13}C) as for organic compound characterization—see above.

The synthesis of all new compounds must be described in detail. Synthetic procedures must include the specific reagents, products and solvents and must give the amounts (g, mmol, for products: %) for all of them, as well as clearly stating how the percentage yields are calculated. They must also include all the characterisation data for the prepared compound or material. For a series of related compounds at least one representative procedure which outlines a specific example that is described in the text or in a table and which

is representative for the other cases must be provided.

3.1.3 Inorganic and Organometallic compounds. A new chemical substance (molecule or extended solid) should have a homogeneous composition and structure. New chemical syntheses must unequivocally establish the purity and identity of these materials.

Where the compound is molecular, minimum standards have been established. For manuscripts that report new compounds or materials, data must be provided to unequivocally establish the homogeneity, purity and identification of these substances. In general, this should include elemental analyses that agree to within $\pm 0.4\%$ of the calculated values. In cases where elemental analyses cannot be obtained (*e.g.* for thermally unstable compounds), justification for the omission of this data should be provided. Note that an X-ray crystal structure is not sufficient for the characterization of a new material, since the crystal used in this analysis does not necessarily represent the bulk sample.

In rare cases, it may be possible to substitute elemental analyses with high-resolution mass spectrometric molecular weights. This is appropriate, for example, with trivial derivatives of thoroughly characterized substances or routine synthetic intermediates. In all cases, relevant spectroscopic data (NMR, IR, UV-vis, *etc.*) should be provided in tabulated form or as reproduced spectra. Again, these may be relegated to the Supplementary Information to conserve journal space. However, it should be noted that in general mass spectrometric and spectroscopic data do not constitute proof of purity, and in the absence of elemental analyses additional evidence of purity should be provided (melting points, PXRD data, *etc.*). Experimental data for new substances should also include synthetic yields, reported in terms of grams or moles, and as a percentage.

Where the compound is an extended solid it is important to unequivocally establish the chemical structure and bulk composition. Single crystal diffraction does not determine the bulk structure. Referees will normally look to see evidence of bulk homogeneity. A fully indexed powder diffraction pattern which agrees with single crystal data may be used as evidence of a bulk homogeneous structure and chemical analysis may be used to establish purity and homogeneous composition.

The synthesis of all new compounds must be described in detail. Synthetic procedures must include the specific reagents, products and solvents and must give the amounts (g, mmol, for products: %) for all of them, as well as clearly stating how the percentage yields are calculated. They must also include all the characterisation data for the prepared compound or material. For a series of related compounds at least one representative procedure which outlines a specific example that is described in the text or in a table and which is representative for the other cases must be provided.

3.1.4 Nano-sized materials (*e.g.* quantum dots, nanoparticles, nanotubes, nanowires). For nano-sized materials it is essential that the authors not only provide detailed characterisation on individual objects (see above) but also a comprehensive characterisation of the bulk composition. Characterisation of the bulk of the sample could require determination of the chemical composition and size distribution over large portions of the sample.

The synthesis of all new compounds must be described in detail. Synthetic procedures must include the specific reagents, products and solvents and must give the amounts (g, mmol, for products: %) for all of them, as well as clearly stating how the percentage yields are calculated. They must also include all the characterisation data for the prepared compound or material. For a series of related compounds at least one representative procedure which outlines a specific example that is described in the text or in a table and which is representative for the other cases must be provided.

3.1.5 Biomolecules (*e.g.* enzymes, proteins, DNA/RNA, oligosaccharides, oligonucleotides). Authors should provide rigorous evidence for the identity and purity of the biomolecules described. The techniques that may be employed to substantiate identity include mass spectrometry, LC-MS, sequencing data (for proteins and oligonucleotides), high field ^1H or ^{13}C NMR,

X-ray crystallography. Purity must be established by one or more of the following: HPLC, gel electrophoresis, capillary electrophoresis, high field 1-H or 13-C NMR. Sequence verification also needs to be carried out for nucleic acid cases involving molecular biology.

For organic synthesis involving DNA, RNA oligonucleotides, their derivatives or mimics, purity must be established using HPLC and mass spectrometry as a minimum.

For new derivatives comprising modified monomers, the usual organic chemistry analytical requirements for the novel monomer must be provided (see 3.1.1. Organic Compounds). It is not however necessary to provide this level of characterisation for the oligonucleotide into which the novel monomer is incorporated.

3.2 General

It is the responsibility of the author(s) to provide the reviewers with the necessary information to evaluate the merit of the manuscript in terms of its scientific content. Failure to provide the necessary experimental evidence and data may result in the manuscript being withdrawn by the Editor.†

4.0 Submissions

4.1 Initial submission

Articles should be submitted using the RSC file upload service, ReSource.‡ A printed copy of the manuscript will **not** be required.

After 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.

4.2 Submission of revised articles and material for proof preparation

Revised manuscripts should be sent to the Editorial Office by file upload *via* ReSource.‡

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

5.0 Administration

Manuscripts should be directed to the appropriate Editor, 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 on-line submission process. Alternatively a completed form, available from the RSC web site,‡ can be sent to the Editor by fax or post.

Authors must provide, in addition to their full contact address, an E-mail address, telephone and fax numbers. They should state explicitly if E-mail and/or fax 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. RSC policy on the initial assessment of submissions, and details of criteria for publication, can be found on ReSource.‡