Chemical Science
Guidelines for Authors[1]
Also see: www.rsc.org/authorguidelines

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1.0 Scope and Standards

Chemical Science is a monthly, peer-reviewed journal for the publication of original research articles of exceptional significance from across the chemical sciences. The journal helps to define the important areas by publishing the most significant cutting edge research. Articles must appeal to the general chemical science community or be of exceptional interest to specialist researchers. Perspectives and Mini Reviews will also be published.

Main research areas include (but are not limited to):

- Organic Chemistry
- Inorganic Chemistry
- Physical Chemistry
- Materials Science
- Nanoscience
- Catalysis
- Chemical Biology
- Analytical Chemistry
- Supramolecular Chemistry
- Computational and Theoretical Chemistry
- Green Chemistry
- Energy and Environmental Chemistry

Authors must include a brief statement justifying why their article should be published in *Chemical Science*.
There are no page or colour charges for articles published in *Chemical Science*.
No work submitted to *Chemical Science* should simultaneously be submitted to or be under current consideration by any other journal.
Articles submitted to *Chemical Science* that are too specialised for the general chemistry audience should be directed to the appropriate RSC specialist title.
Further notes on RSC policy on the initial assessment of submissions and details of criteria for publication can be found on the RSC website.

2.0 Associate Editors

A dynamic and high quality team of Associate Editors will be responsible for the peer review and editorial decisions. The following Associate Editors may be selected as the author's preferred choice at article submission.

1. Stephen Buchwald – Organic Chemistry
2. Thomas Carell – Chemical Biology, Bioorganic Chemistry
3. Christopher C Cummins – Organometallic Chemistry
4. Benjamin Cravatt – Chemical Biology
5. Kazunari Domen – Physical Chemistry, Energy, Surface Science
6. Matthew Gaunt – Organic Chemistry
7. David Leigh – Supramolecular Chemistry
8. Jeffrey Long – Inorganic Chemistry
9. Teri Odom - Nanoscience

[1] 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.

10. Matthew Rosseinsky – Inorganic Materials Chemistry
11. Colin Nuckolls – Organic Materials
12. F. Dean Toste – Organic Chemistry
13. Haw Yang – Physical Chemistry

Please note that it may not always be possible for the author's first choice Associate Editor to be selected. In situations where this is not possible the Editorial Office will assign the most suitable alternative.

3.0 Article types

3.1 Edge Articles

After decades of two main manuscript types (communications and full papers), *Chemical Science* is delighted to introduce a new manuscript type for the publication of frontier and novel research: the Edge Article. *Chemical Science* editors understand that traditional two or three page limits for the dissemination of new research findings is not suitable across all sub-fields of chemistry. Edge Articles are introduced as a manuscript type that fits across all sub-fields. An Edge Article should present a novel piece of scientific research in an exciting, succinct format. Greater than three pages in length, it enables novel research findings to be introduced without the need for abridged discussions or perspectives. As a result, we hope these frontier research studies will be more widely accessible to a larger chemistry audience. However, overtly lengthy introductions and discussion, extensive data, and excessive experimental details and non-experiment based conjecture should not be included. Authors are encouraged to place experimental procedures and characterisation data in the Electronic Supplementary Information (ESI) where appropriate. **Authors must use the template, available from the RSC web site, for preparing their submissions.**

The Society strongly discourages the fragmentation of a substantial body of work into a number of short publications. Unnecessary fragmentation is a valid reason for rejection of manuscripts. All reports measurements should have their uncertainties and limitations clearly stated. Sufficient experimental details should be included such that a scientist skilled in the art would be able to reproduce the results presented (See Supporting Information).

3.2 Mini Reviews

Mini Reviews are short, personal accounts of a new area of research. They can be speculative in nature, putting a new area in perspective. These are normally published by invitation of the *Chemical Science* Associate Editor Board or the Editorial Office. However, suggestions from authors are welcome and enquiries regarding the submission of Mini Reviews should be directed to the Editorial Office. They are typically three to four pages in length.
All Mini Reviews undergo a rigorous and full peer review procedure, in the same way as regular research articles.

3.3 Perspectives

A Perspective should be a concise and critical appraisal of a research area, within the chemical sciences, that will be of interest to the broad general readership of the journal. Perspectives should provide the reader with an overview of a subject and give insight into the field's progression and the potential challenges ahead. Perspectives should be selective rather than comprehensive in their coverage. It is expected that Perspectives will be 10 – 12 pages in length and contain no more than 100 references. Written by leaders in their fields, Perspectives are normally published by invitation of the *Chemical Science* Associate Editor Board. However, suggestions from authors are welcome and enquiries should be directed to the Editorial Office.

To aid the Editorial Office to judge the suitability of a proposed review for the journal, authors may be asked to submit a synopsis. The aim is not to provide an extra burden for the author, but to ensure the article will appeal to the journal's broad readership. **Acceptance of the synopsis by the Editorial Office does not guarantee publication of the final manuscript**. Synopses should include:

- A paragraph explaining the current importance of the field, its implications for the wider scientific community, and the communities of readers who will find the article of interest.

- A structured outline of the review, giving section headings and expanding on each of these.
- A selection of representative references to indicate its breadth and timeliness.

All Perspectives undergo a rigorous and full peer review procedure, in the same way as regular research articles.

4.0 Supporting Information

Experimental information must be provided to enable other researchers to accurately reproduce the work. Figures should include error bars where appropriate, and results should be accompanied by analyses of experimental uncertainty. 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 article. This will depend on the nature of the research being reported.

4.1 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.

4.1.1 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:

- *Analytical:* Elemental analysis (within ±0.4% of the calculated value) is required to confirm ⩾95% sample purity and corroborate isomeric purity. Authors are also encouraged to provide copies of 1H/13C-NMR spectra and/or GC/HPLC traces. 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 SFC/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.
- *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 recrystallisation should also be documented (i.e. solvent, etc.).
- *Spectroscopic:* Mass spectra and a complete numerical listing of 1H/13C-NMR peaks in support of the assigned structure, including relevant 2D NMR and related experiments (i.e. NOE, etc.) is required. 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, 13C 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.

4.1.2 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 characterisation (1H, 13C) as for organic compound characterisation-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.

4.1.3 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 ±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 characterisation 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 characterised 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.

4.1.4 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.

4.1.5 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 1-H 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 4.1.1. Organic Compounds). It is not however necessary to provide this level of characterisation for the oligonucleotide into which the novel monomer is incorporated.

4.2 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.