Journal of Chemical Research: Instructions for Authors

1 General information

The *Journal of Chemical Research* publishes Reviews and Research Papers in experimental chemistry. Papers that are short are welcome, but should not result in fragmentation of publication; they should describe a completed piece of work. *The Journal is not intended as a vehicle for preliminary publications.* The work must meet all the normal criteria for acceptance as regards scientific standards. Papers that contain extensive biological results or material relating to other areas of science may be diverted to more appropriate specialist journals.

The journal is available in print, and online through www.ingentaconnect.com/content/stl/jcr

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http://www.rsc.org/Publishing/ReSourCe/EthicalGuidelines
http://pubs.acs.org/instruct/ethic.html
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2 Editorial procedure

ONLINE SUBMISSION

Authors should check www.jchemres.co.uk to see an electronic copy of a sample paper, and Guidelines for the preparation of papers which are available in both English and Chinese.

All papers must be submitted online via www.jchemres.co.uk

The corresponding author must create an account through which they can submit articles to any Science Reviews 2000 Ltd journal. The author uploads the paper and gives details of all the co-authors on the paper. The submitting author will be the only contact to whom all correspondence regarding referees' comments, editorial matters, and page proofs will be sent, they should ensure that the co-authors are aware of the progress of their paper.

EDITORIAL PROCESS

Receipt of the paper will be acknowledged. The reference number allocated should be quoted in all subsequent correspondence including any resubmission with a new database number. Authors will be able to monitor the progress of their paper by accessing the journal database. As soon as a paper is received it undergoes an initial screening before more extensive editorial review. Papers will be seen by two referees, and their comments will be communicated to the corresponding author by one of the editors through the database. The corresponding author should reply to editorial queries within a month otherwise any revision will be treated as a new submission. The present rate of acceptance is about 30%.

The corresponding author will receive details by E-mail for downloading their page proofs. These proofs should be checked carefully and corrections returned to the Editorial Office by the date indicated. *If no corrections are received by the date specified, the publisher will assume that no corrections are required.*

The corresponding author will be given a link to download a copy of their paper from which reprints may be generated. The corresponding author will be required to agree to an exclusive copyright license held by Science Reviews 2000 Ltd.

FORMAT OF PAPERS

Text

Papers should be written in English. Papers in which the standard of English is inadequate will not be considered. Authors whose first language is not English are advised to have their manuscript checked before submission. They may also purchase a "Language polishing service" via http://www.charlesworthauthorservices.com/~ASH

i. Title.
ii. Names of authors, with one forename for each given in full. Indicate by * the author who will deal with correspondence. This should be the same as the submitting author.
iii. Address(es) of authors. Include any postal or zip codes and the E-mail address of the corresponding author.
iv. A graphical abstract to be used for the contents.
v. The abstract must be independent of the text of the paper and detailed in terms of compounds or reagents for abstraction on the internet. Compounds should be identified by name and not by their structure number. Only standard abbreviations for reagent and solvents should be used.
vi. Up to eight specific keywords.
vii. Text. Microsoft Word files not less than 11 point size, single column, double spaced (*i.e.* not more than eight lines of typing to a depth of 50mm), unjustified, and without hyphenation. PDF format should not be used. Auto-referencing features that bury references within the text should not be used. Graphics and Tables should be included in the same file as the text and must be accompanied by suitable legends. Tables: use either the word processor's table editor or tabs for formatting (not a mixture). Where possible, tables concerning related compounds should be constructed using a generic formula and R', R" *etc.* to denote substituents rather than drawing separate structural formulae.
viii. Further relevant material can be added as Electronic Supplementary Information (ESI). Editors may ask for the data used for the identification of known compounds or the data used in the characterisation of a series of closely related compounds to be presented as ESI. The methods used for the preparation of known compounds, particularly if they involve minor variations of the literature procedure, may be presented as ESI. Large tables of data should be included as ESI. The material in the ESI should be listed at the end of the paper.

Graphics

Any graphics must fit a one- or two-column format with maximum width 8 cm or 17 cm. Formulae should be numbered sequentially using bold Arabic numerals: **1**, **2**, *etc*. Authors should provide either TIFF, EPS, ChemDraw, or Word files. The required settings in formula drawing programs are Helvetica 9 point font, bond length 0.43 cm, and bond width 0.056 cm (the RSC setting in ChemDraw). Formulae deviating from this standard may be returned for redrawing.

References

References should be numbered individually in the text as superscripts, after any punctuation, and collected at the end of the paper.

Each paper which is referenced must be given a separate reference number.

All notes must be incorporated into the text.

The last author's name must be preceded by 'and'.

Journal abbreviations as listed in http://images.webofknowledge.com/WOK46/help/WOS/A_abrvjt.html should be used.

1. D.N. Smith and A.D. Bond, *J. Org. Chem*., 1983, **19**, 5997.
2. O. Arnet, P. Sanda and J.R. Stewart, *Aspects of aromaticity*, eds M. Charton and F. Hudson. Academic Press, New York, 1996. Vol. 1, pp. 185-189.
3. C. Cai, P.K. Hu and J. Yao, *J. Chem. Res.*, 2012, doi: XXXXXXXXXXXXXXX available online at http://www.ingentaconnect.com/content/stl/jcr (epub prior to publication).

Referees may ask to see the manuscript of papers that are described as 'in the press' or papers that have been published in relatively inaccessible journals.

3 Experimental requirements

Authors must highlight any possible health and safety problems that could arise from compounds or procedures used in their work. Authors are warned that the use of domestic microwave ovens for chemical purposes can be unreliable and potentially hazardous. Where a domestic oven has been used a note to this effect should be added to the general experimental section.

Details should be given of any instruments and manufacturer that are used, and the source of any spectroscopic or analytical services.

Convincing evidence of both purity and identity must be given for all new compounds; this will normally require good elemental analysis, which should be quoted to 0.01%, the accuracy should normally be to within ±0.4%. The elemental composition may be defined by a high resolution mass spectrum, but this must be accompanied by additional evidence of purity. Compounds that have been prepared before should be given the appropriate references. Relevant physical data, such as the melting point, should be quoted for comparison.

^{1}H NMR shifts should be quoted to two decimal places. The multiplicity, relative integrals, and *J* values should be quoted to one decimal place and assignments given where possible. ^{13}C chemical shifts should be quoted to one decimal place. Other numerical data should not be quoted to a greater precision than the measurements warrant. Only IR peaks which characterise the functional groups of the compounds should be quoted. For low resolution mass spectra, the eight major peaks, with the relative intensities, should be given. In general, a detailed discussion of the fragmentation pattern should not be included. Editors or referees may ask to see copies of spectra or of the original results of analyses.

4 X-Ray crystallographic work

A brief mention of a crystallographic determination may be given in the title. Reference should be made to it in the abstract, without including cell dimensions and other crystal data.

The experimental details of data collection and structure analysis should be concise where routine procedures are used. Brief descriptions of any non-routine procedures should be given. The method used for structure solution and the treatment of H atoms where appropriate should be stated.

A conventional line drawing of the structure should normally be included, except in the simplest cases, and one perspective diagram (or stereo pair) if appropriate. Packing diagrams should not be included unless required to illustrate a specific chemical point. The atom-numbering scheme should be shown in one of the diagrams. Each atom of the asymmetric unit should be assigned an Arabic numeral in parentheses following the chemical symbol: C(2), O(12), *etc.*

The description of the structure may be given in textual or tabular form; the latter is more appropriate if several structure determinations are being reported. Any special details, such as hydrogen bonding, should be mentioned. If significant comment is made on the structures, tables of selected bond parameters with estimated standard deviations can be included. Such a table should be restricted to significant dimensions only (*e.g.* it is rarely necessary to include data for phenyl rings). Differences from expected norms should be noted. The experimental section of the paper should include the following:

1. The crystal data, including the formula, Mr
2. The space group, cell dimensions and volume
3. The number of formula units in the unit cell (Z)
4. The wavelength of the radiation and the linear absorption coefficient (u)
5. The diffractometer that was used and the range for collecting data (q, *h, k, l*)
6. The total number of reflections that were collected, the number of independent reflections and the number that were used in the structure determination.
7. The programmes that were used, including appropriate citations.
8. The R factors and residual electron density, peak and hole.
9. Details of where the data have been deposited and the accession number.

The *Journal of Chemical Research* expects that the data will have been submitted to the Cambridge Crystallographic Data Centre (CCDC) or equivalent centre. A check list of items for deposition is available from the (CCDC) either by E-mail (to fileserv@ccdc.cam.ac.uk with the one-line message sendme depform) or through http://www.ccdc.cam.ac.uk/; the form can be saved as a simple text file).

The data that are deposited must include:

(1) A table of *final fractional atomic coordinates.*
(2) Any *calculated coordinates* (*e.g.* of hydrogen).
(3) A full list of *bond lengths and angles* with estimated standard deviations.
(4) A full list of *displacement parameters* in the form *Bij* or *Uij* (in Å^2 or pm^2)

Tables of *structure factors* (F0, Fc) should not be sent, but retained by the authors so that they can be made available to the referees if requested. The CIF and a CheckCIF report must be submitted with the paper. Referees will require that a satisfactory response is given to any significant alerts that the report has raised.

5 Reviews

Short reviews are published. These are normally commissioned, but authors who are interested in contributing such a review should contact one of the Editors. Reviews should be between 8,000 and 13,000 words in length. Authors will be remunerated at a rate of £40 ($60) per printed page up to a maximum of £240 per review.

Guidelines for the Preparation of Chemistry Papers for Publication

These notes have been prepared by the editors of the *Journal of Chemical Research* but they apply equally to any journal in the same field. We receive many papers which report good chemistry but are not acceptable because the presentation would need too much editing to bring them up to a publishable standard. We have therefore prepared these notes, which supplement our Instructions for Authors (http://www.sciencereviews2000.co.uk/downloads/instructions/jcr.pdf), and which we hope will be useful to inexperienced authors and will reduce the number of papers which are rejected or returned to the authors for rewriting.

Research papers

The fragmentation of work into a series of short papers is strongly discouraged. This is particularly the case when a series of related papers are submitted to different journals making it difficult for readers to follow the progress of the work. A more substantial paper will have a larger impact and be more widely cited. Papers are unlikely to be accepted if they only describe a change in reaction conditions such as carrying out a well-established reaction under microwave irradiation or in an ionic liquid and provide only a small advantage and make no contribution to our understanding of the chemistry of the reaction. Papers on topics such as environmental or biochemical analysis or which contain a substantial quantity of biological or kinetic data, or theoretical calculations may also not be accepted if they are more appropriate to a specialist journal.

Accuracy

The publication of scientific work rests on trust concerning the accuracy, honesty and novelty of the work that is being reported. Editors may ask for the original data such as the printed output from elemental analysers, or NMR and IR spectra, to support claims in the paper, and authors who do not provide such information on demand, or who violate in other ways these conditions of trust, may be blacklisted and find it difficult to publish their work in future. Authors should ensure that their co-authors are in agreement with the publication of the work. Difficulties have arisen when a junior member of a team has submitted work without the permission of the leader of the team.

Instructions for authors

Before preparing their manuscript authors MUST consult the journal's 'Instructions for Authors'. These are usually published in the January issue of the journal and are available on line (at http://www.sciencereviews2000.co.uk/downloads/instructions/jcr.pdf). These instructions contain important information on the style of papers, the conventions that are used and the procedure for submitting manuscripts. Details of the style and format of papers can be gained from previous issues of the Journal.

Text style

The title for a paper should be short, accurate and informative. Lengthy titles, and those which claim more than is substantiated by the text of the paper, are likely to be changed or rejected. The titles of papers, the contents of the abstracts and the 'keywords' form the basis from which a number of electronic databases and information retrieval systems are constructed. Authors should ensure that these are sufficiently accurate and contain the specific key words which would enable their work to be retrieved electronically by search engines.

The careful wording of an abstract is of major importance in enabling others to decide whether or not to read the full paper. The abstract should be essentially independent of the main paper. Reference to structure numbers in the main paper should be avoided. A graphical abstract should also be provided.

The address which is given for the authors must be that at which the work was carried out. When a senior author has moved to another department, that address should also be cited. An E-mail address is essential for correspondence concerning the paper.

The text of a paper usually falls into four sections: • introduction • results and discussion • experimental • references Some papers may also have electronic supplementary information (ESI) which is available on line but which is not printed.

The *introduction* should state why the work was carried out and its objectives. It should contain sufficient

background information together with the associated references to enable the reader to put the work into its context. However, many authors include too much irrelevant information and material that is already widely known. In many cases, reference to a readily accessible review accompanied by a brief summary of the prior work and the present state of knowledge together with a short justification of the research, is adequate.

The *results and discussion* section should describe the methodology that was used and the significant data on which the conclusions were based. References should be given to appropriate literature analogies. Where a novel method of carrying out a transformation is described, care should be taken to demonstrate its significant advantages over the existing methodology possibly by quoting suitable comparisons or by indicating a situation where the current method does not work.

Where results are given in a table, this should contain the relevant characterizing information. For example if a series of known compounds have been prepared by a novel method, comparison data such as melting point together with a literature value and the appropriate reference should be cited. Where a new compound is described as part of a synthetic sequence, sufficient spectroscopic and chemical evidence should be cited to establish its structure and exclude possible alternative structures. Where two-dimensional NMR spectra are used, the resonances associated with the key interactions should be identified. In the case of a complex structure this can sometimes be done with a diagram.

Although in the published order of a paper, the experimental section usually follows the discussion; in writing the paper it may be helpful to prepare a flow diagram and the experimental section before writing the discussion. In this way, the salient evidence that needs to be highlighted in the discussion may become clear. Furthermore consistency between the two parts of the paper is more easily achieved. Only the data that are necessary to establish a scientific point should be given in the discussion section. The full characterization data for a new compound should be given in the experimental section. Where abbreviations are used both in the experimental section and in the text, authors should check that these follow the common practice. Lists of standard abbreviations are published by the Royal Society of Chemistry. Non-standard abbreviations must be defined.

The *experimental* part of the paper should contain a section of general experimental details listing the spectroscopic and analytical equipment that was used and where the analyses were carried out. The description of the specific experiments should contain sufficient information to enable the reader to repeat the experiments. Inadequate or incomplete submission of experimental information is a major cause of papers being queried or rejected. Authors must consult the 'Instructions for Authors' to see the format for the presentation of these data.

In listing the characterizing data for a new compound the usual order is: name of compound, yield, m.p. (or b.p.), IR, NMR, MS and analysis, with the molecular formula. Attention should be paid to the number of significant figures that are quoted and to the use of units. Known compounds must be referenced and comparison data quoted whilst new compounds must be fully analysed either by a combustion analysis or by a high resolution mass spectrometric analysis of the molecular ion. The IR and NMR spectra of new compounds must also be given. In listing IR data only those absorptions that are characteristic of particular structural features (*e.g.* OH, C=O or C=C) should be quoted. The presentation of ^{1}H NMR data is often incomplete. Wherever possible, authors should give the coupling constants. Not only are these important in establishing stereochemistry but they also play a role in assigning resonances and in distinguishing between isomers. Mutually coupled protons must have matching *J* values. Ambiguities which can arise from taking data from computer printouts must be resolved. There have been many examples of papers which have been queried by the referees and returned for revision because spectra have been determined on high-field instruments and yet the coupling constants were not given or where resonances were unsatisfactorily described as multiplets. The solvent in which the NMR spectra were determined should be given. In the case of 13C NMR spectra it is helpful to distinguish between resonances arising from methyl, methylene, methine and quaternary carbons. Where the 13C NMR spectra for a series of compounds have been recorded, tabulating the data may reveal changes in the position of resonances that reflect the structural changes and indeed these changes may provide further confirmatory evidence for the conclusions that have been drawn.

Where possible, new compounds should be given their systematic names. A compound is considered to be new if it has not been prepared before or, if has been prepared before, it was not adequately purified or characterised or was assigned an erroneous structure. The quantities of materials that have been used in the experiments should follow the name of the substance to which they refer, *i.e*. “water (15 mL)” rather than “15 mL of water”.

Authors should note the different uses of the comma, semicolon, and colon in listing data. Foreign words and Latin abbreviations are given in italics.

In describing biological material the scientific names of genera and species are italicized. Where plant material is reported as the source of a new product, the origin of the plant material and the place where a voucher specimen has been deposited, should be given. Where possible, authors should also quote the name of the person that identified the plant. Where a micro-organism is used, the culture collection where the strain is deposited should be given.

Serious hazards should be identified. Papers may be rejected if they advocate the use of particularly hazardous procedures.

X-Ray crystallographic data should be deposited with the Cambridge Crystallographic Data Centre before the paper is submitted, and the accession number should be quoted.

The “Instructions for Authors” give details of the data which should be included in the paper. If the R values are higher than normal, the reason for this should be given as this may preclude some uses of the data. A paper should not contain conclusions that rest on unpublished crystallographic data.

The format for references is given in the Instructions for Authors. In order to facilitate the use of online “Crossref” electronic referencing, each reference number should cite only one paper. The sub-division of references into (a) and (b) should not be used. Footnotes should not be included in the references but given separately in the text. All the authors of a paper should be cited. The use of *et al*. in the reference list is not permitted. The format for references is given in the Instructions for Authors. The abbreviations for journals can be found at http://images.webofknowledge.com/WOK46/help/WOS/A_abrvjt.html
Careful consideration should be given to the choice if the generic names for groups of compounds, and to the *keywords* used for the description of particular novel techniques.

Electronic supplementary information appears only on the web, and enables authors to enhance their paper with, for example, full colour diagrams, 3D molecular models, and bulky experimental data. This material is usually refereed by not edited.

Diagrams

Diagrams should normally fit a single column of a double-column page. It is often helpful to use a single formula to represent a series of related compounds. This can be done by using a series of independently varying R^1, R^2, and R^3 groups. Where these are also linked in a flow diagram or reaction scheme, it is important to ensure that the arrows linking structures are consistent with the inter-relationships that are reported in the experimental section. Ambiguities can arise if not all
the transformations have been carried out.

English

Papers are published in English. For many authors English is not their first language. Authors are strongly advised to ask an English-speaking colleague to check their papers. A language polishing service is available to purchase via
http://www.charlesworth-group.com/our-services/author-services/language-polishing.html
There are a number of simple rules to avoid misunderstandings. Do not use long and complicated sentences. Use one sentence for one subject. Keep the tenses consistent and use simple words rather than long words. A common fault is to omit 'a' or 'the' before a noun. The incorrect and superfluous use of adjectives and adverbs is another common fault. Always be concise in expression. Some common faults which can obscure the

meaning, include the use of a number of adjectives in front of a noun. A series of subordinate clauses within a sentence can also confuse the reader. Phrases with a low information content can often be abbreviated to a single word. The careful choice of words is very important. Some pairs of words such as absorb and adsorb, or affect and effect, are easily confused.

Plagiarism

Plagiarism, the unattributed copying of another author's work and ideas, is a serious offence. This can apply to the copying of specific passages in the introduction and the discussion. “Self- plagiarism” – the re-use of introductory material from another paper, or the recycling of experimental details – is also an objectionable practice and may lead to the black-listing of authors by the Journal.

See: http://publicationethics.org/resources/international-standards

Submissions

Articles should be submitted to *Journal of Chemical Research* as a conventional single column manuscript with lines that are double-spaced; other journals may require the paper to be prepared on a template which they provide. Pages should be numbered. Diagrams, structures and tables should be submitted on separate pages. Problems often arise in the electronic transmission of manuscripts when authors attempt to embody these within the text.