# **Journal of Chemical Research: Instructions for Authors**

## **1** General information

### Introduction

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, and 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.

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

Papers are published in the English language. Authors whose first language is not English are advised to have their manuscript checked before submitting their paper. Papers in which the standard of English is inadequate will not be considered.

Scientific publishing is based on trust, and editors, publishers, and readers have the right to expect that papers are free from fraudulent data, plagiarised material, or duplicate publications. The Journal adheres to the code of ethics which is maintained by the major chemical societies; further details may be found on the web at <a href="http://www.rsc.org/Publishing/ReSourCe/">http://www.rsc.org/Publishing/ReSourCe/</a> EthicalGuidelines/and at <a href="http://pubs.acs.org/instruct/ethic.html">http://pubs.acs.org/instruct/ethic.html</a>

#### Administration

Manuscripts should be submitted online to www.jchemres.co.uk

# 2 Presentation of papers

The style in which manuscripts are published is best seen from recent examples in the Journal. An electronic copy of a sample paper and Guidelines for the preparation of papers are available online on www.jchemres.co.uk

Typescripts should be prepared in double spacing (*i.e. not more than eight lines of typing to a depth of 50 mm*). The format should be as follows:

- i. Title.
- Names of authors, with one forename for each given in full. Indicate with an asterisk (\*) the name of the author who will deal with correspondence.
- iii. Address(es) of authors. Include any postal or zip codes and the E-mail address of the author who will deal with correspondence.
- iv. A graphical abstract to be used for the contents.
- v. The abstract must be independent of the text of the paper and sufficiently detailed in terms of compound or reagents for the purpose of abstraction on the internet. Compounds should be identified by name and not by their structure number within the paper. Only standard abbreviations for reagent and solvents should be used.
- vi. Up to eight keywords.
- vii. Text. Microsoft Word or WordPerfect files, double-spaced, unjustified, ranged left, and without hyphenation. Autoreferencing features that bury references within the text should not be used. Graphics: TIFF or EPS format. Tables: use either the wordprocessor's table editor or tabs for formatting (not a mixture).
- viii Further relevant material can be added as Electronic Supplementary Information (ESI). Editors may ask for the data which has been 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 that have been used for the preparation

An E-mail address of one correspondent must be provided for notification of page proof upload and for receiving editorial comments. The editorial office will deal only with this correspondent.

Receipt of the paper will be acknowledged, and a reference number allocated that should be quoted in all subsequent correspondence. Authors will be able to monitor the progress of their paper by accessing the journal database.

The present rate of acceptance is about 40%.

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

Papers will be seen by two referees, and their comments will be communicated to the corresponding author by one of the Editors. The corresponding author is expected to reply to editorial queries within a month otherwise any revision will be treated as a new submission. The corresponding author will have the opportunity to download a copy of their paper via the internet from which reprints may be generated. The corresponding author will be required to sign an exclusive copyright licence.

of known compounds, particularly if they involve minor variations of the literature procedure, may also be considered for presentation as ESI. Large tables of data should also be included as ESI. A list of the material in the ESI should be given in the published paper.

Colour can be used but authors will be charged, before publication, £100 per printed page on which colour is used. However, colour may be used free of charge within the ESI and in the online version of the article. Any graphics must fit a one- or two-column format with maximum width 8 cm or 17 cm. Formulae should be numbered sequentially using Arabic numerals: (1), (2) *etc.* Authors should provide either TIFF, EPS, ChemDraw, or Word files. The required settings in formulae drawing programs are: Arial 7 point font, bond length 0.43 cm/13 points, and bond width 0.016 cm/0.6 points (the RSC setting in ChemDraw).

References should be numbered individually in the text as superscripts, after any punctuation, and collected at the end of the paper in the following style. In order to make articles published on-line more accessible and available for crossreferencing purposes, references should not be separated into parts (a), (b) *etc.* and all notes should be incorporated into the text. The last author's name must be preceded by 'and'. Journal abbreviations as listed in <u>http://www.rsc.org/publishing/</u> <u>resource/authorguidelines/authoringtools/journalabbreviations/</u> <u>index.asp should be used.</u>

- 1. D.N. Smith and A.D. Bond, J. Org. Chem., 1983, 19, 5997.
- 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 print).

### 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 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  $\pm 0.4\%$ . The elemental composition may be defined by a high resolution mass spectrum,

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.

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.

but this must be accompanied by additional evidence of purity. Key compounds that have been prepared before should be given the appropriate reference and relevant physical data, such as the melting point, should be quoted for comparison.

<sup>1</sup>H NMR shifts should be quoted to two decimal places. The multiplicity, relative integrals, and *J* values should be quoted and assignments given where possible. <sup>13</sup>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. Editors or referees may ask to see copies of spectra or of the original results of analyses.

The R factors and residual electron density, peak and hole.
Details of where the data has been deposited and the accession number.

#### Submission of crystallographic data via electronic mail

Authors are encouraged to submit all supplementary crystallographic data as an ASCII file *via* electronic mail. The preferred format is the Crystallographic Information File (CIF). Authors should combine multiple data sets for a given manuscript into a single file. The individual structures in the combined file must be separated from each other by the sequence "#=END" at the beginning of a line. Authors must identify which manuscript the electronic file is associated with by entering the name of the manuscript at the top of the electronic file.

It is expected that the data will have been submitted to the Cambridge Crystallographic Data Centre (CCDC) or equivalent centre.

The information required for deposition includes:

- A check list of items for deposition. This is available from the (CCDC) either by E-mail (to fileserv@ccdc. cam.ac.uk with the one-line message sendme depform) or via the World Wide Web (the CCDC Home Page is <u>http://www.ccdc.cam.ac.uk/; the form</u> can be saved as a simple text file).
- (2) A table of *final fractional atomic coordinates*.
- (3) Any calculated coordinates (e.g. of hydrogen).
- (4) A full list of *bond lengths and angles* with estimated standard deviations.
- (5) A full list of *displacement parameters* in the form *Bij* or *Uij* (in Å<sup>2</sup> or pm<sup>2</sup>)

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. Where possible a Check CIF report should be provided.

### 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 2,000 and 5,000 words in length. Authors will be remunerated at a rate of £40 (\$60) per printed page up to a maximum of £240 per review.