Author Guidelines

RSC Publishing

What to send and when

At Submission

Please consult individual journal guidelines for details of any additional required files.

In general, initial manuscript submissions to the RSC should consist of:

- Manuscript text as PDF, Word or plain text (submissions to *ChemComm* must use the RSC template). TeX files are accepted for submissions to *PCCP* and *Soft Matter* and must be accompanied by a PDF of the manuscript.
- Graphics (either included within or at the end of the text).
- A graphical and textual abstract for the Table of contents entry.
- Any Electronic Supplementary Information.
- Any crystallographic CIF files in plain text format only, as well as CheckCIF files for each crystal structure. A file listing potential referees may be submitted.
- A covering letter, including a justification of the importance of the work.

At Revision

For manuscripts that need revision, or have been accepted without further changes, the following files are required:

- Manuscript text as Word or plain text files. Tables included in the manuscript must be submitted as text files.
- Graphics saved separately. ChemDraw files are particularly useful when enhancing the online Prospect version of an article.
- A graphical and textual abstract for the Table of Contents pages.
- Electronic Supplementary Information.
- Any revised crystallographic CIF files in plain text format only.
- A covering letter, detailing the changes that have been made to the manuscript and responding to all comments of the referees.

Proof Correction

When sending your proof corrections to the editorial office, please provide the following:

- A list of corrections.
- Any revised graphics, saved separately.
- Any new or revised supplementary data.

*Please **do not** send:*

- A modified version of the proof PDF file.
- A revised manuscript.

How to submit

Initial submission

Articles should be submitted using the RSC file upload service at http://mc.manuscriptcentral.com/rsc.

On submitting their manuscripts, authors are encouraged to supply the names and addresses of 2-3 potential referees.

The submissions service allows for up to five files to be uploaded at one time. Alternatively a ZIP file containing up to 20 files can be uploaded. All files relating to a single manuscript should be uploaded simultaneously during one transaction. Files uploaded separately will result in more than one manuscript number being assigned.

After submission your file will be acknowledged as soon possible. Authors should contact the editorial office if they have not received an acknowledgement within 4 working days. Authors should not forward an additional copy of their manuscript by post or e-mail to avoid duplicate entries of their manuscripts by the editorial office.

Submission of revised manuscripts

Revised manuscripts should be submitted using RSC file upload service at http://mc.manuscriptcentral.com/rsc.

Authors should ensure that files submitted at this stage contain the final version of their manuscript. Proof corrections should only correct errors from the Production process and should not be used to make general changes to the text.

We will try to use the supplied data in our production process, but mathematical equations and tables in particular may be re-keyed by the typesetter.

Proofs for correction

PDF proofs for correction are sent by e-mail to the corresponding author. Please note that authors are responsible for the final proof-reading of manuscripts. It is therefore imperative that authors check the proofs very carefully. Particular attention should be paid to numerical data both in the tables and text. Proof corrections should be returned to the editorial office within 48 hours of receipt. Corrections at this stage should be minor and not involve extensive changes. All corrections must be sent at the same time. Papers are published as Advance Articles on the web as soon as possible after proof corrections are received from the authors. Late corrections cannot be incorporated after publication of the Advance Article.

Licence to publish

All authors submitting work for publication are required to agree a Licence to Publish. Authors submitting online will be asked to agree a Licence to Publish as part of the submission process. Alternatively, a downloadable PDF version is available, which can be completed and forwarded by email, post or fax to the editorial office.

Preparing your article for submission

Please also read the Ethical guidelines document
http://www.rsc.org/Publishing/Journals/guidelines/EthicalGuidelines/index.asp

1.0 Organisation of material

Article templates can be found at:
http://www.rsc.org/Publishing/Journals/guidelines/AuthorGuidelines/AuthoringTools/Templates/index.asp

1.1 Full papers

Full papers present original high quality primary research that has not been previously published. Extensions on work that has appeared in print in a short form such as a Communication are normally acceptable.

1.1.1 Title
A paper should have a short, straightforward title directed at the general reader. Lengthy systematic names and complicated and numerous chemical formulae should therefore be avoided where possible. The use of non-standard abbreviations and symbols in a title is not encouraged. Please bear in mind that readers increasingly use search engines to find literature; recognisable, searchable terms should be included in the title where possible. Brevity in a title, though desirable, should be balanced against its accuracy and usefulness. The use of Series titles and Part numbers in titles of papers is discouraged. Instead these can be included as a footnote to the first page together with a reference (reference 1) to the preceding part. When the preceding part has been submitted to the RSC but is not yet published, the paper reference number should be given.

1.1.2 Author names
Full names for all the authors of an article should be given. To give due acknowledgement to all workers contributing to the work, those who have contributed significantly to the research should be listed as co-authors. On submission of the manuscript, the corresponding author attests to the fact that those named as co-authors have agreed to its submission for publication and accepts the responsibility for having properly included all (and only) co-authors. If there are more than ten co-authors on the manuscript the corresponding author should provide a statement to specify the contribution of each co-author. The corresponding author signs a copyright licence on behalf of all the authors.

1.1.3 Table of contents entry
This entry should include a colour image (no larger than 8 cm wide and 4 cm high), and 20-30 words of text that highlight the novel aspects of your work.

Graphics should be as clear as possible, simple schematic diagrams or reaction schemes are preferred to ORTEP-style crystal structure depictions and complicated graphs, for example. The graphic used in the Table of Contents entry need not necessarily appear in the article itself. Authors should bear in mind the final size of any lettering on the graphic. For examples, please see the online version of the appropriate journal.

1.1.4 Abstract
Every paper must be accompanied by a summary (50-250 words) setting out briefly and clearly the main objects and results of the work; it should give the reader a clear idea of what has been achieved. The summary should be essentially independent of the main text; however, names, partial names or linear formulae of compounds may be accompanied by the numbers referring to the corresponding displayed formulae in the body of the text. Please bear in mind that readers increasingly use search engines to find literature; recognisable, searchable terms and keywords should be included in the abstract to enable readers to more effectively find your paper.

1.1.5 Introduction
This should give clearly and briefly, with relevant references, both the nature of the problem under investigation and its background.

1.1.6 Results and discussion
It is usual for the results to be presented first, followed by a discussion of their significance. Only strictly relevant results should be presented and figures, tables, and equations should be used for purposes of clarity and brevity. The use of flow diagrams and reaction schemes is encouraged. Data must not be reproduced in more than one form, *e.g.* in both figures and tables, without good reason.

1.1.7 Experimental
Descriptions of experiments should be given in detail sufficient to enable experienced experimental workers to repeat them.

The degree of purity of materials should be given, as should the relative quantities used. Descriptions of established procedures are unnecessary. Standard techniques and methods used throughout the work should be stated at the beginning of the section. Apparatus should be described only if it is non-standard; commercially available instruments are referred to by their stock numbers (*e.g.* Perkin-Elmer 457 or Varian HA-100 spectrometers). The accuracy of primary measurements should be stated. Unexpected hazards encountered during the experimental work should be noted. In general there is no need to report unsuccessful experiments. Authors are encouraged to make use of ESI for lengthy synthetic sections.

Any unusual hazards inherent in the use of chemicals, procedures or equipment in the investigation should be clearly identified.

In cases where a study involves the use of live animals or human subjects, the author should include a statement that all experiments were performed in compliance with the relevant laws and institutional guidelines, and also state the institutional committee(s) that have approved the experiments. They should also include a statement that informed consent was obtained for any experimentation with human subjects. Referees may be asked to comment specifically on any cases in which concerns arise.

1.1.8 Conclusion
This is for interpretation and to highlight the novelty and significance of the work. The conclusions should *not* summarise information already present in the text or abstract.

1.1.9 Acknowledgements
Contributors other than co-authors may be acknowledged in a separate paragraph at the end of the paper; acknowledgements should be as brief as possible. All sources of funding should be declared.

1.1.10 Dedications
Personal dedications of an appropriate nature may be included as a footnote to the title of the paper. Dedications for significant birthdays (from 60 years onwards) and *in memoriam* dedications would be considered appropriate. Other forms of dedication may require approval of the relevant journal editor.

1.1.11 Bibliographic references and notes
These should be listed at the end of the manuscript in numerical order.

1.2 Communications

Communications contain novel scientific work of such importance and interest that rapid publication is required. Individual Communications should be as brief as possible. Depending on the journal in question, a page limit may apply and authors may be required to use the Communication template, available from the RSC web site, for preparing their submissions. Most journals also request authors to provide a statement explaining the reasons why they feel that publication of their work as a Communication is justified. Formatting should be as for Full Papers, except for the following topics.

1.2.1 Text
No section headings are used in Communications. Brief details of key experiments are permitted but lengthy introductions and discussion, extensive data, and excessive experimental details and conjecture should not be included. The experimental evidence necessary to support a communication should be supplied for the referees to aid in their assessment of the work and for eventual publication as Electronic Supplementary Information. Description of routine procedures should not be included.

1.2.2 Figures and tables
These should be kept to a minimum and will in general only be published if they are essential to understanding the Communication.

1.3 Reviews
Review articles are normally the result of an invitation from the editorial office. Please consult the editor of the journal in question if you are interested in writing a review.

2.0 Style and presentation

2.1 Brevity

Papers should be written clearly and concisely. Repetition or embellishment with unnecessary words or phrases should be avoided. Excessive use of diagrams and duplication of data in text, tables and figures is discouraged.

2.2 Grammar and spelling

Standard English or American spelling is used but consistency should be maintained within a paper.

2.3 Abbreviations

The use of common or standard abbreviations is encouraged. If non-standard abbreviations must be used these should be defined at the first use.

2.4 Use of italics

Foreign words and phrases and Latin abbreviations are given in italics: *e.g.*, *in toto*, *in vivo*, *ca.*, *cf.*, *i.e.*

In the names of chemical compounds or radicals italics are used for prefixes (other than numerals or symbols) when they define the positions of named substituents, or when they define stereoisomers: other prefixes are printed in roman. (*Note:* Initial capital letters are not to be used with italic prefixes or single-letter prefixes: full stops are not to be associated with letter prefixes.) For example, *o-, m-* and *p*-nitrotoluenes, but *ortho*-, *meta*- and *para*- compounds (*o*-, *m*- and *p*- are used only with specific names; *ortho*-, *meta*- and *para*- are used with classes), *N*,*N*-dimethylaniline, *trans*- and *cis*-bis(glycinato)platinum(II), *gem*- and *vic*-diols, benzil *anti*-oxime.

The names of journals or their abbreviations are set in italics.

3.0 Graphics

3.1 Preparation of graphics

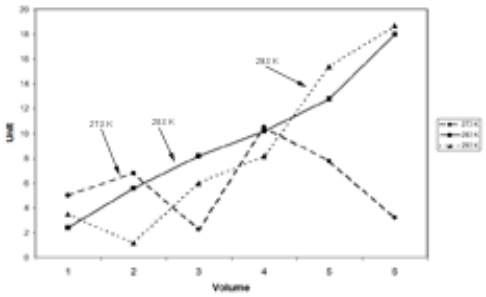
Artwork should be submitted at its ***final size*** so that reduction is not required. The appearance of graphics is the responsibility of the author.

- Graphics should fit within either single column (8.3 cm) or double column (17.1 cm) width, and must be no longer than 23.3 cm.
- Graphical abstracts should be no larger than 8 x 4 cm.
- Schemes and structures should be drawn to make best use of single and double column widths.

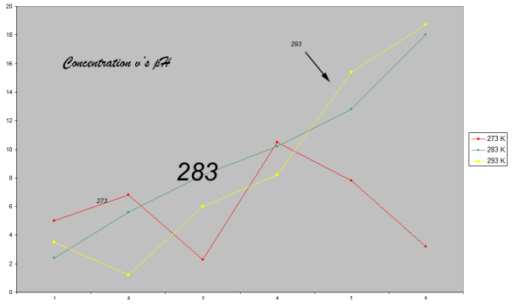
3.1.1 Graphs

i) bad examples

Example A



Example B



Both examples above (A and B) will not reproduce well due to the following problems:

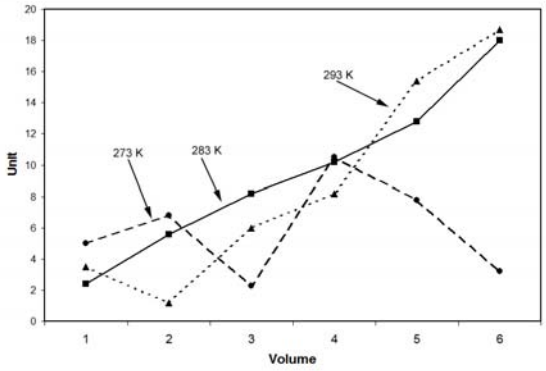
- Example A has not been provided at the required resolution and size so it will appear unclear and blurry in the final article.

- Example B:
  - yellow lines will not appear faint
  - red and green are bad choices, with low visibility, particularly to colour-blind people
  - in graphs, broken, dashed and dotted lines should be used rather than colour
  - faint writing, overlapping writing and unusual fonts should be avoided

In addition, graphs from instruments should be re-plotted using appropriate graphing software. ASCII (txt) files can usually be exported from the instrument to the software to create a clear, easily readable plot.

ii) good example

Example C



Example C will reproduce well:

- Image is legible and clear to the reader as it has been provided at the correct size [single column (8.3 cm) or double column (17.1 cm) width]
- Lines should be black, of an adequate and even thickness (e.g. 1 pt) and curves should be smooth
- Broken, dashed, dotted lines and simple geometric symbols: such as □■▲○● should be used rather than colour

- Lettering used in graphics should be legible at the required size (e.g. 7 point Arial font or Helvetica if Arial is unavailable)
- The format of units in graphics should conform to IUPAC convention and be consistent with those used in the paper
- Insets in images should be avoided where possible. However, if insets are used there is no need to shrink down the size of the text, axes labels and symbols in the inset. These should be the same size as in the main graph so that they are readable.

3.2 Photographs

- Photographs should be provided at the best resolution available (minimum 300 dpi) at a reasonable size (unlike Photo A). Biography photographs should be 40 mm x 50 mm. All other photographs should conform to the regular figure sizes (see section 3.1).
- Reproduction of black and white photos is far superior to that of colour photos

Photo A

Photo B

3.3 Chemical Structures

Structural formulae should ideally be prepared with chemistry drawing software (*e.g.* ChemDraw, ChemWindows, ISIS/Draw), using the settings below.

- Chain bond angle = 120°
- Fixed bond angle = 15°
- Bond length = 0.43 cm *or* 12.2 pt
- Bond width = 0.016 cm *or* 0.5 pt
- Bold bond width = 0.056 cm *or* 1.6 pt
- Double bond space = 20% of bond length
- Stereo bond width = 0.056 cm *or* 1.6 pt
- Hash spacing = 0.062 cm *or* 1.8 pt
- Captions/atom labels = Arial/Helvetica, 7 pt

3.3.1 ChemDraw files and ChemSpider

Wherever possible, please send all ChemDraw files with the final version of your manuscript. We can use good, clear, chemical drawings to highlight your research and make it more discoverable via the RSC's ChemSpider database (http://www.chemspider.com/).

These chemical drawings need not be the ones that are used in the finished article. For guidance on how to best prepare your ChemDraw files for ChemSpider see http://www.chemspider.com/gettingstarted.aspx

3.4 Crystal structure images

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 clearly shown in one of the diagrams.

3.5 Colour figures

Colour figure reproduction is normally provided free of charge if the use of colour enhances the scientific understanding of the figure, and it is this aspect that is considered by the editor when determining whether figures should be reproduced free in colour or not. If the use of colour is approved by the editor, authors should provide colour artwork for publication and colour will be provided free of charge in the print, PDF and HTML versions of the article. The figure captions and the text of the article may mention the colour in the figure if required. In general colour is not required for the following types of figures: simple line graphs and similar figures where points can be marked with symbols, labelled ORTEP plots, schematic diagrams, organic reaction schemes, images that have been falsely coloured (*e.g.* AFM images), photographs of people and equipment and histograms. Please note that this list is not comprehensive.

It is possible to reproduce colour artwork free of charge in the PDF and HTML versions of an article. If this option is appropriate the authors should provide only colour artwork; however the figure caption and text of the article must not contain any reference to colour. The print article will be in black and white - the colour artwork provided by the author will be converted to greyscale by the RSC. It is important therefore that the exact same figure and accompanying text makes sense in both the black and white and colour versions. Only the PDF and HTML article will contain the colour artwork.

If the author prefers colour where the scientific understanding of the figure is not enhanced, then the author will be charged a partial contribution to the additional production costs. Authors should contact the editorial office for further details. Colour artwork should be provided and the print, PDF and HTML versions of the article will appear in colour. The figure captions and the text of the article may mention the colour in the figure if required.

Specific advice may be obtained from the editorial office of the journal to which the contribution is to be submitted. The editor's decision on the use of colour is final.

3.6 Journal covers

Authors who wish to have their artwork featured on a journal cover should contact the editorial office of the journal to which the article is being submitted. A contribution to the additional production costs will be requested. Use of such artwork is at the editor's discretion; the editor's decision is final.

Examples of previous journal covers can be viewed *via* the relevant journal homepages.

4.0 Characterisation of new compounds

4.1 General guidance

It is the responsibility of authors to provide fully convincing evidence for the homogeneity and identity of all compounds they claim as new, or known compounds made by a new method. Evidence of both purity and identity is required to establish that the properties and constants reported are those of the compound with the new structure claimed.

A compound is considered as new (a) if it has not been prepared before, (b) if it has been prepared before but not adequately purified, (c) if it has been purified but not adequately characterized, (d) if, earlier, it has been assigned an erroneous constitution, or (e) if it is a natural product isolated or synthesized for the first time.

Referees will assess, as a whole, the evidence in support of the homogeneity and structure of all new compounds. No hard and fast rules can be laid down to cover all types of compound, but evidence for the unequivocal identification of new compounds should wherever possible include good elemental analytical data; an accurate mass measurement of a molecular ion does not provide evidence of purity of a compound and must be accompanied by independent evidence of homogeneity. Where elemental analytical data cannot be obtained, appropriate evidence which is convincing to an expert in the field may be acceptable, but authors should include, for the referees, an explanation of the special nature of their problem. More detailed guidelines for authors submitting to *ChemComm* or *Organic & Biomolecular Chemistry* can be found the individual journal summary guidelines.

Spectroscopic information necessary to the assignment of structure should be given. Just how complete this information should be must depend upon the circumstances; the structure of a compound obtained from an unusual reaction or isolated from a natural source needs much stronger supporting evidence than one derived by a standard reaction from a precursor of undisputed structure. Authors are reminded that full spectroscopic assignments may also be treated as Supplementary Data (see Section 7) where their importance does not justify their inclusion in the published paper.

Particular care should be taken in supporting the assignments of stereochemistry (both relative and absolute) of chiral compounds reported, for example by NMR spectroscopy, X-ray crystallography, polarimetry or correlation with known compounds of undisputed configuration. In cases where mixtures of isomers are generated (*e.g. E/Z* isomers, enantiomers, diastereoisomers), the constitution of the mixture should usually be established using appropriate analytical techniques (*e.g*. NMR spectroscopy, GC, HPLC) and reported in an unambiguous fashion. In the case of asymmetric reactions in which enantiomeric mixtures are prepared, the direct measurement of the enantiomer ratio and its reporting expressed as an enantiomeric excess (ee) is recommended, and is preferred to (less reliable) polarimetry methods.

4.2 Characterisation within chemical biology

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.

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.

4.3 Presentation of experimental data

Data associated with particular compounds should be listed after the name of the compound concerned, following the description of its preparation. **The following is suggested as the order in which the most commonly encountered data for a new compound should be cited**: yield, melting point, optical rotation, refractive index, elemental analysis, UV absorptions, IR absorptions, NMR spectrum, mass spectrum. Appropriate formats for the citation of each are as follows.

4.3.1 Yield

In parentheses after the compound name (or its equivalent). Weight and percentage are separated by a comma, *e.g*. the lactone (7.1 g, 56%).

4.3.2 Melting point
In the form mp 75 °C (from EtOH), *i.e*. the crystallization solvent in parentheses. If an identical mixed melting point is to be recorded, the form mp and mixed mp 75 °C is appropriate.

4.3.3 Optical rotation
The *units* should be stated in the preamble to the Experimental section, *e.g*. $[\alpha]_D$ values are given in 10^{-1} deg cm^2 g^{-1}. Shown in the form $[\alpha]_D^{22}$ -22.5 (*c* 0.95 in EtOH), *i.e*. concentration and solvent in parentheses.

4.3.4 Refractive index
Given in the form n_D^{22} 1.653.

4.3.5 Elemental analysis
In the presentation of elemental analyses, both forms (Found: C, 63.1; H, 5.4. $C_{13}H_{13}NO_4$ requires C, 63.2; H, 5.3%) and (Found: C, 62.95; H, 5.4. Calc. for $C_{13}H_{13}NO_4$: C, 63.2; H, 5.3%) are acceptable. Analyses are normally quoted to the nearest 0.1%, but a 5 in the second place of decimals is retained. For identification purposes for new compounds, an accuracy to within ±0.3% is expected, and in exceptional cases, to within ±0.5% is required. If a molecular weight is to be included, the appropriate form is: [Found: C, 63.1; H, 5.4%; M (mass spectrum), 352 (or simply M^+, 352). $C_{13}H_{13}NO_4$ requires C, 63.2; H, 5.3%; M, 352].

4.3.6 UV absorptions
These are given in the form λ_{max}(EtOH)/nm 228 (ε/dm^3 mol^{-1} cm^{-1} 40 900), 262 (19 200) and 302 (11 500). Inflections and shoulders are specified as 228infl or 262sh. Alternatively the following form may be used: λ_{max} (EtOH)/nm 228, 262 and 302 (ε/dm^3 mol^{-1} cm^{-1} 40 900, 19 200 and 11 500). log ε may be quoted instead of ε.

4.3.7 IR absorptions
As follows: ν_{max}/cm^{-1} 3460 and 3330 (NH), 2200 (conj. CN), 1650 (CO) and 1620 (CN). The type of signal (s, w, vs, br) can be indicated by appended letters (*e.g*. 1760vs).

4.3.8 NMR data
For all spectra δ values should be used, with the nucleus indicated by subscript if necessary (*e.g*. δ_H, δ_C). A statement specifying the units of the coupling constants should be given in the preamble to the Experimental section, *e.g*. *J* values are given in Hz. Instrument frequency, solvent, and standard should be specified. For example: δ_H(100 MHz; $CDCl_3$; Me_4Si) 2.3 (3 H, s, Me), 2.5 (3 H, s, COMe), 3.16 (3 H, s, NMe) and 7.3-7.6 (5 H, m, Ph). A broad signal may be denoted by br, *e.g*. 2.43 (1 H, br s, NH). Order of citation in parentheses: (i) number of equivalent nuclei (by integration), (ii) multiplicity (s, d, t, q), (iii) coupling constant, *e.g*. $J_{1,2}$ 2, J_{AB} 4, (iv) assignment; italicisation can be used to specify the nuclei concerned (*e.g*. CH_3CH_2). The proton attached to C-6 may be designated C(6)H or 6-H; the methyl attached to C-6, 6-Me or C(6)Me. Mutually coupled protons in ^{1}H NMR spectra must be quoted with precisely matching *J* values, in order to assist thorough interpretation. In instances of any ambiguities when taking readings from computer print-outs, mean *J* values should be quoted, rounded to the nearest decimal point.

4.3.9 Mass spectrometry data
Given in the form: *m*/*z* 183 (M^+, 41%), 168 (38), 154 (9), 138 (31) *etc*. The molecular ion may be specified as shown if desired. Relative intensities in parentheses (% only included once). Other assignments may be included in the form *m*/*z* 152 (33, M - CH_3CONH_2). Metastable peaks may be listed as: M* 160 (189 ⟶ 174), 147 (176 ⟶ 161), *etc*. The type of spectrum (field desorption, electron impact, *etc*.) should be indicated. Exact masses quoted for identification purposes should be accurate to within 5 ppm (EI and CI) or 10 ppm (FAB or LSIMS).

4.3.10 Magnetic couplings
To avoid ambiguity, where magnetic couplings are reported, the Hamilton convention used should be included.

4.3.11 Literature citations
If comparison is to be made with literature values, these should be quoted in parentheses, *e.g*. mp 157 °C (from chloroform) (lit.,[19] 156 °C), or ν_{max}/cm^{-1} 2020 and 1592 (lit.,[24] 2015 and 1600).

4.3.12 Experiments involving microorganisms
For work involving microorganisms, sufficient detail should be provided to identify the species being used.

5.0 Bibliographic references, notes and footnotes

Bibliographic reference to the source of statements in the text is made by use of *superior numerals* at the appropriate place (e.g., Wittig[3]). The reference numbers should be cited in the correct sequence through the text (including those in tables and figure captions, numbered according to where the table or figure is designated to appear). Please do not use Harvard style for references. The references themselves are given at the end of the final printed text along with any Notes. The names and initials of all authors are always given in the reference; they must not be replaced by the phrase *et al*. This does not prevent some, or all, of the names being mentioned at their first citation in the cursive text: initials are not necessary in the text.

Notes or Footnotes may be used to present material which, if included in the body of the text, would disrupt the flow of the argument but which is, nevertheless, of importance in qualifying or amplifying the textual material. Footnotes are referred to with the following symbols: †, ‡, §, ¶, ‖ *etc.* Alternatively the information may be included as Notes (end-notes) to appear in the Notes/references section of the manuscript. Notes should be numbered using the same numbering system as the bibliographic references.

5.1 Journals

The style of journal abbreviations to be used in RSC publications is that defined in Chemical Abstracts Service Source Index (CASSI). See http://www.cas.org/expertise/cascontent/caplus/corejournals.html

If you cannot locate an authoritative abbreviation for a journal, and if it is not obvious how the title should be abbreviated, please cite the full title.

Bibliographic details should be cited in the order: year, volume, page.

Where page numbers are not yet known, articles should be cited by DOI (Digital Object Identifier), *e.g.* A. R. Jones, *Dalton Trans.*, 2005, DOI: 10.1039/B503459J.

5.2 Books
J. Barker, in *Catalyst Deactivation*, ed. B. Delmon and C. Froment, Elsevier, Amsterdam, 2nd edn., 1987, vol. 1, ch. 4, pp. 253-255.

5.3 Patents
Br. Pat., 357 450, 1986. *US Pat*., 1 171 230, 1990.

5.4 Reports and bulletins, *etc.*
R. A. Allen, D. B. Smith and J. E. Hiscott, *Radioisotope Data*, UKAEA Research Group Report AERE-R 2938, H.M.S.O., London, 1961.

5.5 Material presented at meetings
H. C. Freeman, Proceedings of the 21st International Conference on Coordination Chemistry, Toulouse, 1980.

5.6 Theses
A. D. Mount, Ph.D. Thesis, University of London, 1977.

5.7 Reference to unpublished material
For material presented at a meeting, congress or before a Society, *etc*., but not published, the following form is used:
A. R. Jones, presented in part at the 28th Congress of the International Union of Pure and Applied Chemistry, Vancouver, August, 1981.
For material accepted for publication, but not yet published, the following form is used:
A. R. Jones, *Dalton Trans.*, 2003, DOI: 10.1039/manuscript number
is used for RSC journals, and:
A. R. Jones, *Angew. Chem.*, in press.
is used for non-RSC journals. If DOI numbers are known these should be cited in the form recommended by the publisher.
For material submitted for publication but not yet accepted the following form is used:
A. R. Jones, *Angew. Chem.*, submitted.
For personal communications the following is used:
G. B. Ball, personal communication.
If material is to be published but has yet to be submitted the following form is used:
G. B. Ball, unpublished work.

Reference to unpublished work should not be made without the permission of those by whom the work was performed.

6.0 Guidelines for the publication of X-ray crystallography

These guidelines are divided into separate sections for single crystal and powder diffraction data and apply to submission to any RSC journal.

6.1 Single crystal data

Authors should submit their work in CIF (Crystallographic Information File) format as it will facilitate the rapid processing of their manuscript.

In addition, authors should provide the checkcif report for their submitted CIFs. The checkcif reports are available *via* the International Union of Crystallography's free checkcif service. Any 'level A' alerts in the report should be explained in the submission details for the article.

The Cambridge Crystallographic Data Centre (CCDC) has a freely available programme (enCIFer) which allows users to add RSC required information to CIF files *via* a user-friendly graphical interface and can be used to provide a CIF in a suitable format for the IUCr's checkcif service.

Related Links

checkCIF http://checkcif.iucr.org/
CIF checking service of the International Union of Crystallography

Cambridge Crystallographic Data Centre (CCDC) http://www.ccdc.cam.ac.uk/
The CCDC is dedicated to the advancement of chemistry and crystallography for the public benefit through providing high-quality information services and software.

International Union of Crystallography (IUCr) http://www.iucr.org/
The IUCr is a member of the International Council for Science (ICSU) and exists to serve the world community of crystallographers.

enCIFer http://www.ccdc.cam.ac.uk/free_services/encifer/
CIF checking, editing and visualisation software from the CCDC

The following information must be included in the CIF for assessment and deposition:

- 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 refinement, which should include the following data:

- Chemical formula and formula weight (M)
- Crystal system
- Unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, temperature
- Space group symbol (if non-standard setting give related standard setting)
- No. of formula units in unit cell (Z)
- Number of reflections measured, number of independent reflections, R_{int}, theta and index (hkl) range
- Final R value(s) and whether for all or observed data
- Method of determination of unit cell dimensions
- Type of filter or monochromator used
- Type and wavelength of radiation used
- Calculated density (D_c)
- Method of refinement, whether refinement carried out on F or F^2, treatment of hydrogen atoms
- Details of weighting scheme used
- No. parameters refined and any constraints or restraints applied
- Definition of R and wR, final value of wR, with a statement of whether unobserved data were included
- Goodness-of-fit (S) value, maximum/minimum residual electron densities, average and maximum shift/error
- Programs or packages and computers used (with references)
- Flack or Rogers parameter (if appropriate)

The CIF format has data names that correspond to these items.

Tables of structure factors (F_o, F_c) should not be sent, but copies should be retained by the authors so that they may be made available *via* the editorial office if requested.

The RSC has a CIF Data Importer available for authors. More details can be found at: http://www.rsc.org/Publishing/Journals/guidelines/AuthorGuidelines/AuthoringTools/CIFDataImporter/CIFFormatForCIfDataImporter.asp

6.1.2 Information for inclusion in manuscript

Abstract. Reference should be made to the crystal structure in the abstract. However it should not contain cell dimensions and other crystal data.

Full papers. Where appropriate, the description may be given in textual or tabular form, although the latter is more appropriate if several structure determinations are being reported in one paper. A table of selected bond lengths and angles, with estimated standard deviations should be restricted to significant dimensions only. Average values may be given (with a range of e.s.d.s) for chemically equivalent groups or for similar bonds.

If the procedures for data collection and structure analysis were routine, their description should be particularly concise. When the analysis was not of a routine nature, the authors should briefly detail the procedures used.

Communications. Details of the data collection and CCDC numbers should be given in a footnote or in the References/Notes section. Where given, selected bond lengths and angles, with estimated standard deviations, should be included in the figure caption and be restricted to significant dimensions only.

The following data must be presented in the manuscript if there is significant discussion of the crystallography:

- Chemical formula and formula weight (*M*)
- Crystal system
- Unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, temperature
- Space group symbol (if non-standard setting give related standard setting)
- No. of formula units in unit cell (*Z*)
- Number of reflections measured and/or number of independent reflections, R_{int}
- Final *R* values (and whether quoted for all or observed data)
- Flack or Rogers parameter (if appropriate)

The following example demonstrates the application of the recommendations in the preceding sections in a full paper. For a communication, the headings should be omitted.

> Single crystals of [Pd{C(CO_2Me)[C(CO_2Me)C(CO_2Me)=C(CO_2Me)C(CO_2Me)=C(CO_2Me)]C_6H_3[CH(Me)NH_2]-2-NO_2-5}Br] **4** were recrystallised from dichloromethane, mounted in inert oil and transferred to the cold gas stream of the diffractometer.
>
> **Crystal structure determination of complex 4**
>
> **Crystal data.** $C_{28}H_{31}BrCl_4N_2O_{14}Pd$, M = 947.66, orthorhombic, a = 11.096(1), 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, 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).

6.1.3 Post submission

Supplementary crystallographic data will be deposited by the RSC with the Cambridge Crystallographic Data Centre (CCDC) as part of the assessment process. Each structure will be assigned a separate CCDC number that will be quoted in the subsequent crystallographic report.

Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and organometallic compounds will be entered into the Cambridge Structural Database. Post-publication requests for individual data sets should be directed to the CCDC.

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 Deposition Number(s) provided in the RSC crystallographic report should be quoted in that publication, and the CCDC advised of the new journal and the appropriate reference. Data will then enter the appropriate database as described above.

6.2 Powder diffraction data

If available, authors may submit supplementary crystallographic data as a Crystallographic Information File (CIF) file *via* the RSC submissions service. 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 when they submit the file by entering the name of the manuscript at the top of the electronic file. The information required for deposition includes:

- 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 refinement.
- Profile difference plots for all analyses. Where a range of similar analyses are presented a minimum number of representative plots may be given

6.2.1 Unrefined powder diffraction data

Unrefined powder diffraction data should normally only be reported where the data form 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 in either textual or tabular format. The latter presentation is more appropriate if several powder diffraction studies are being reported in one paper.

- Diffractometer name and model
- Radiation wavelength (Å)
- Temperature of data collection
- Unit cell dimensions (Å or pm, degrees), 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 Electronic Supplementary Information scheme.

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

6.2.2 Refined powder diffraction data (where atomic coordinates have been determined)

Description
If the procedures for data collection and structure analysis were routine, their description should be particularly concise. When the analysis has not been of a routine nature, the authors should briefly detail the procedures used. In most cases a table of atomic coordinates may be provided which should give details of occupancies that are less than unity. Anisotropic thermal parameters may be included if they form an important aspect of the study. Selected bond lengths and angles, with estimated standard deviations, should be given.

Illustrations
For Rietveld refinements, an observed + calculated + difference profile plot should normally 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.

The following information should be given in the manuscript:

- Diffractometer name and model
- Radiation wavelength (Å)
- Temperature of data collection
- Step size
- Chemical formula and formula weight (M)
- Unit cell dimensions (Å or pm, degrees)
- Space group
- Z
- Number of reflections
- Final R values (R_{wp}, R_{exp} and R_I) and method of background treatment

6.3 Referencing structures in previously published communications or unpublished work

6.3.1 Crystallographic work published in a preliminary communication

If an author does not wish to discuss the structure again at any length in the corresponding full paper, he/she may refer back to the original communication. However if the structure is discussed in detail in the full paper, the data should be re-presented in full and will be re-published if considered necessary.

6.3.2 Unpublished crystallographic work

There may be cases when an author wishes to publish a paper in which the result of a crystal structure determination is discussed, but where he/she does not wish to include details or extensive discussion. In these cases, it may be appropriate provided that it does not lead to unnecessary fragmentation. The editor will have the final decision. However the author must provide, as supplementary information, sufficient data to allow a reader to make sure that the point made is correct, and coordinates *etc*. will be deposited at the Cambridge Crystallographic Data Centre (or the Fachinformationszentrum Karlsruhe). The brief description of the determination should be referenced as 'unpublished work'.

6.4 Using 3D Chime figures

2D ball-and-stick or ORTEP-style plots have been the traditional way of illustrating the 3D structure in a crystal for many years. However, it can sometimes be particularly difficult to communicate a complex three-dimensional structure in this way. With the increasing popularity of electronic publishing, new and improved methods that enable a 3D representation of crystal structures are now available. 3D diagrams have several advantages over their 2D counterparts that appear in print:

- Fully interactive - figures can be rotated and resized on-screen, giving viewers a better opportunity to understand complex structures
- Unlimited use of full colour - different atom types can be easily distinguished and different sections of a structure can even be highlighted to show complex structural motifs
- Structures can be displayed in a variety of styles - from simple ball-and-stick to van der Waals space filling views

By making full use of the RSC's free Electronic Supplementary Information (ESI) service and the free Chime plug-in, these new methods of electronic publishing can be easily utilised by authors to better communicate their results to readers.

Related Links
Chime Plug-In http://www.symyx.com/downloads/index.jsp
Chime lets scientists view chemical structures from within popular Web browsers, Java Applets, and Java applications.

6.6 Protein crystallography

For details on this, see section 7.2.2

7.0 Supplementary Data

7.1 Electronic Supplementary Information

7.1.1 Introduction

The RSC's Electronic Supplementary Information (ESI) service is a free facility that enables authors to enhance and increase the impact of their articles. Authors are encouraged to make the most of the benefits of publishing supplementary information in electronic form. Such data can take full advantage of the electronic medium, allowing use of full colour diagrams, 3D molecular models and movies.

Authors can also improve the readability of their articles by placing appropriate material, such as repetitive experimental details and bulky data, with the ESI service. All information in the ESI service is also fully archived.

It is intended that the ESI system should make full use of developing file types to allow authors to present their data in the most useful and interesting ways possible. If you are providing an unusual file type, please provide the editorial office with details of any additional software that would be required to view the files. Such software should be available freely, preferably via the web.

When preparing their ESI data files, authors should keep in mind the following points:

- Supplementary data is peer-reviewed and should therefore be included with the original submission.
- ESI files are published 'as is'-editorial staff won't normally edit the data for style or content
- Data is only useful if readers can access it - use common, widely known file formats
- Large files may prove difficult for users to download and access

7.1.2 Text and graphics

The preferred format for ESI comprising text and graphics is Microsoft Word. Publishing staff will convert Word files to PDF before publication as this format can be accessed easily and reliably on most computing platforms using the freely available Adobe Acrobat Reader. If other formats are submitted they will also usually be converted to PDF files prior to publication.

7.1.3 Spectral files

In addition to including spectra in Word files, we encourage authors to make this data available to the community by submitting JCAMP-DX files of their spectra which we will deposit with ChemSpider.

ChemSpider is a freely available database that brings together any chemical information (names, chemical suppliers, spectra, patents and literature citations) and links them all to a chemical structure, allowing you to search records by name, synonym, structure and more.

See http://www.jcamp-dx.org/

7.1.4 Multimedia files

We welcome submission of multimedia files (including videos and animations) alongside articles for publication. Videos are an excellent medium to present elements of your work that can be difficult to communicate in words alone. [Please note that any videos of general interest are shared with the wider community via the RSC Journals YouTube channel. Please notify the editorial team if you prefer for your video(s) not to be uploaded to YouTube.]

If you submit a multimedia file alongside your paper please refer to it in your paper to draw it to the reader's attention. Also please see the section on Submitting Multimedia files

Format

Acceptable formats for video or animation clips include .WMV, .AVI, .MOV and .MPG

Your video or animation clips will be viewed via our Web server, and we need to consider the needs of users with dial-up internet connections so that your work can be made available to the widest possible readership.

Please minimize file sizes where you can, by considering the following points:

- 640 x 480 pixels is the recommended maximum frame size.
- Many packages output 30 frames per second (fps) as standard, but you can specify a lower frame rate. This may not noticeable affect the quality of your video but can reduce the file size.
- Use a 256 colour palette if that is suitable for the presentation of the material.
- Our recommended maximum file size is 5MB.

Please consider the use of lower specifications for all these points if the material can still be represented clearly.

If your video is very short (i.e., several seconds long) then it is recommended that you put this onto a loop and repeat the film a few times to provide a more detailed view.

Submitting Multimedia files
Upload your video online, together with your manuscript under the category "Electronic Supplementary Material" and please supply:

- Clear file name for your video
- Short descriptive title for the video which can be used when uploading the video onto a streaming channel
- A video legend of approx 30 words long this caption must be provided to aid discoverability.
- 5 – 10 keywords which can be used to tag the video, the more accurate the tags are the better discoverability videos will have.

7.1.5 3D files and spectral data files
We offer a service that enables the 3D visualisation of complex molecules. This is made possible by using the PDB identification code to generate an image using FirstGlance in Jmol.

Related Links
Adobe Acrobat Reader http://get.adobe.com/uk/reader/
PDF files require the Adobe Acrobat Reader which can be downloaded free of charge
FirstGlance in Jmol http://firstglance.jmol.org/
A simple tool for macromolecular visualization

7.2 Externally deposited data

7.2.1 Crystallographic data

Please see the X-ray crystallography section of the guidelines for full details.

7.2.2 Macromolecular structure and sequence data

Novel macromolecular structures and newly reported nucleic acid or protein sequences and microarray data must be deposited with the appropriate database. Articles will not be published until the relevant 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.

We recommend authors refer to the Minimum Information for Biological and Biomedical Investigations (MIBBI) Portal for prescriptive checklists for reporting biological and biomedical research where applicable. Microarray data should be MAIME compliant.

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. Authors are encouraged to pre-submit their data to the PDB and obtain a wwPDB validation report for their structure to check the structure(s). 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 as summary data tables in the manuscript, or as ESI.

Reference may also be made to data deposited with PubChem. Suitable links should be provided as footnotes to the text of the article.

7.2.3 System models

The Systems Biology Markup Language (SBML) is a computer-readable format for representing models of biochemical reaction networks. SBML is applicable to metabolic networks, cell-signaling pathways, regulatory networks, and many others.

We encourage authors to prepare models of biochemical reaction networks using the Systems Biology Markup Language (SBML) and to deposit the model with the BioModels database. Authors can submit datasets in SBML formats when they are available for publication as supplementary data.

Related Links

- **Worldwide Protein Data Bank** http://www.wwpdb.org/
A repository for the processing and distribution of 3D biological macromolecular structure data
- **Nucleic Acids Database** http://ndbserver.rutgers.edu/
A repository of three-dimensional structural information about nucleic acids
- **National Center for Biotechnology Information (GenBank)** http://www.ncbi.nlm.nih.gov/
NCBI develops software tools and supports research in computational molecular biology
- **DNA Data Bank of Japan** http://www.ddbj.nig.ac.jp/
DDBJ provides an online DNA database and tools for data retrieval and analysis
- **UniProt** http://www.ebi.ac.uk/uniprot/
An annotated protein sequence database established in 1986
- **EMBL Nucleotide Sequence Database** http://www.ebi.ac.uk/embl/
(also known as EMBL-Bank) constitutes Europe's primary nucleotide sequence resource.
- **Protein Information Resource (Protein Sequence Database)** http://pir.georgetown.edu/
Public resource of protein informatics to support genomic and proteomic research
- **ArrayExpress** http://www.ebi.ac.uk/arrayexpress/
A public repository for microarray data, storing MIAME-compliant data in accordance with MGED recommendations
- **Gene Expression Omnibus (GEO)** http://www.ncbi.nlm.nih.gov/geo/
A gene expression/molecular abundance repository
- **MIAME** http://www.mged.org/Workgroups/MIAME/miame.html
Minimum information about a microarray experiment
- **PubChem** http://pubchem.ncbi.nlm.nih.gov/
Providing information on the biological activities of small molecules
- **BioMagResBank** http://www.bmrb.wisc.edu/
A repository for data from NMR spectroscopy on proteins, peptides and nucleic acids.
- **MIBBI** http://www.mibbi.org/index.php/Main_Page
Minimum Information for Biological and Biomedical Investigations
- **BioModels Database** http://www.ebi.ac.uk/biomodels-main/
A data resource that allows biologists to store, search and retrieve published mathematical models of biological interests.
- **SBML** http://sbml.org
Systems Biology Markup Language. Information on the SBML project which helps develop a variety of software packages for SBML.