

Article Layout

Guidelines for Layout of Articles for Submission†

Also see: www.rsc.org/authorguidelines

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1.0 Organization of material

Every latitude, consistent with brevity, in the form and style of papers is permitted, and no rigid pattern for either is prescribed. **The suggestions outlined here are for guidance only.**

1.1 Full articles

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. 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 the Series title and Part number 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 Society but is not yet published, the paper reference number should be given.

† For more detailed information on this topic, as well as links to useful websites and software resources, see: <http://www.rsc.org/authorguidelines>.

1.1.2 Author names. Full names for all the authors of an article should be given; initials should not be used.

1.1.3 Graphical contents entry. Graphics are included in the contents list. The format incorporates, a small graphic (maximum size 8 cm wide × 4 cm high) alongside one sentence of text, which should be presented in such a way as to encourage further perusal of the article, by highlighting the novelty and main feature(s) of interest; excessive lists of results and, in particular, cumbersome formulae should therefore be avoided.

In view of the space available 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 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 of graphical contents entries check the online version of the appropriate journal.

1.1.4 Summary. 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.

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.

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.

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's Editorial Board.

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

1.2 Communications

Individual articles should be as brief as possible; depending on the journal in question, a page limit may apply. Formatting should be as for Full Articles, except for the following topics.

1.2.1 Summary. This is restricted to one sentence of text.

1.2.2 Article. No section headings are used in Communications. Brief details of key experiments are permitted and should include the amounts of reagents used in chemical reactions. Extensive spectroscopic and other supporting data are not required, but authors are encouraged to supply such data as Electronic Supplementary Information to aid the referees in their assessment of the work. Description for routine procedures should *not* be included.

1.2.3 Notes and bibliographic references. These should not be extensive and inclusion of 5–10 references is recommended.

1.2.4 Figures. These should be kept to a minimum bearing in mind the restrictions to the length of most Communications.

2.0 Style and presentation

2.1 Brevity

For reasons of economy, brevity in the presentation of papers is essential. Authors should note that the following practices are likely grounds for rejection of a manuscript, or acceptance only after substantial revision.

- Unnecessary division of work into separate parts of a series of papers.
- Submission of fragmentary work which can be included in a larger article.
- Undue elaboration of hypotheses.
- Over-detailed and verbose exposition of ideas.
- Excessive use of diagrams; for example, a straight-line plot can be adequately expressed as an equation together with, if necessary, a table of deviations.
- Duplication of data in text, tables and figures, *etc.*
- Descriptions of slight variations of essentially the same technique.

2.2 Linguistic and typographical conventions

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

2.2.2 Abbreviations. The use of common or standard abbreviations is encouraged.

2.2.3 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 periodicals or their abbreviations are set in italics.

2.2.4 Headings.

- (a) Main sections (Experimental, Results and discussion, *etc.*): side-heading, bold, first initial capital letter only, no final fullstop.
- (b) Main side-heading: bold, first initial capital letter only, no final fullstop.
- (c) Subsidiary side-heading: bold, first initial capital letter only, final fullstop.
- (d) Further subdivision: italic, first initial capital letter only, final fullstop.

For example:

Experimental

Preparation of the thiolate complexes

Bis(benzenethiolato)bis(dimethyldithiocarbamato)[*N,N*-dimethylhydrazido(2-)]molybdenum(VI) 10. Method 1. Benzenethiol (1 g) was added to . . .

3.0 Presentation of experimental data

3.1 Physical characteristics of compounds

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.

3.1.1 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%).

3.1.2 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.

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

3.1.4 Refractive index. Given in the form $n_{\text{D}}^{22} 1.653$.

3.1.5 Elemental analysis. In the presentation of elemental analyses, both forms (Found: C, 63.1; H, 5.4. $\text{C}_{13}\text{H}_{13}\text{NO}_4$ requires C, 63.2; H, 5.3%) and (Found: C, 62.95; H, 5.4. Calc. for $\text{C}_{13}\text{H}_{13}\text{NO}_4$: 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 $\pm 0.3\%$ is expected, and in exceptional cases, to within $\pm 0.5\%$ 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). $\text{C}_{13}\text{H}_{13}\text{NO}_4$ requires C, 63.2; H, 5.3%; M, 352].

3.1.6 UV absorptions. These are given in the form $\lambda_{\text{max}}(\text{EtOH})/\text{nm}$ 228 ($\epsilon/\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$ 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 ($\epsilon/\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$ 40 900, 19 200 and 11 500). $\log \epsilon$ may be quoted instead of ϵ .

3.1.7 IR absorptions. As follows: $\nu_{\max}/\text{cm}^{-1}$ 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).

3.1.8 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 ^1H 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.

3.1.9 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: $\text{M}^* 160 (189 \rightarrow 174)$, $147 (176 \rightarrow 161)$, 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).

3.1.10 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 $\nu_{\max}/\text{cm}^{-1}$ 2020 and 1592 (lit.,²⁴ 2015 and 1600).

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

3.1.12 A typical experimental section. The paragraph below exemplifies many of the points made in the preceding sections.

(*E,E*)-Undeca-3,8-diene-1,11-diol **16**

A solution of the undeca-3,8-diyne-1,11-diol (2 g, 11 mmol) in tetrahydrofuran (2 cm^3) was added cautiously dropwise over 5 min to a stirred solution of lithium aluminium hydride (8.3 g, 22 mmol) in tetrahydrofuran (200 cm^3) at 0 °C. The mixture was heated under reflux in an atmosphere of nitrogen for 20 h, after which it was cooled and quenched by careful addition of saturated aqueous sodium sulfate. The mixture was acidified with dilute hydrochloric acid (100 cm^3) and then extracted with diethyl ether (4 \times 100 cm^3). The combined extracts were dried and evaporated under reduced pressure to leave a yellow oil, which was purified by column chromatography on silica using diethyl ether as eluent to give the dienediol **16** (1.9 g, 95%) as a colourless oil (Found: C, 71.5; H, 11.4. $\text{C}_{11}\text{H}_{20}\text{O}_2$ requires C, 71.7; H, 10.9%); $\nu_{\max}(\text{film})/\text{cm}^{-1}$ 3342, 1777, 1711, 968 and 766; δ_{H} (250 MHz; CDCl_3 ; Me_4Si) 1.45 (2 H, quintet, J 7.4, $\text{CH}_2\text{CH}_2\text{CH}_2$), 1.65 (2 H, br s, OH), 2.03 (4 H, dt, J 6.6 and 7.4, $2 \times \text{CH}_2\text{CH}=\text{CH}$), 2.27 (4 H, dt, J 7.6 and 6.3, $2 \times \text{CH}_2\text{CH}=\text{CH}$), 3.63 (4 H, t, J 6.3, $2 \times \text{C H}_2\text{OH}$) and 5.34–5.61 (4 H, m, $2 \times \text{CHCH}$); δ_{C} (67.8 MHz; CDCl_3 ; Me_4Si) 29.3 (t), 32.3 ($2 \times$ t), 36.2 ($2 \times$ t), 62.3 ($2 \times$ t), 126.6 ($2 \times$ d) and 133.4 ($2 \times$ d); m/z (EI) 154.1334 ($\text{M}^+ - \text{CH}_2\text{O}$. $\text{C}_{10}\text{H}_{18}\text{O}$ requires 154.1358), 135 (7%), 125 (7), 107 (24), 98 (38) and 81 (100).

3.2 Characterisation of new compounds

It is the responsibility of authors to provide fully convincing

evidence for the homogeneity and identity of all compounds they claim as new. 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. In preliminary communications compounds are often recorded with limited characterizing data; in spite of (c) above later preparations of such compounds are not considered as new if the properties previously reported are confirmed; the same applies to patents.

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 e.g. HPLC. Low-resolution mass spectrometry must be treated with even more reserve in the absence of firm evidence to distinguish between alternative molecular formulae. 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.

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 always be treated as Supplementary Data (see Section 3.5) 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, GLC, 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.

3.3 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.

The homogeneity of oligomeric compounds (peptides, saccharides, nucleotides etc.) should be determined by HPLC analyses or by other appropriate analytical methods (e.g. capillary electrophoresis) with a purity of not less than 95%.

4.0 Bibliographic references, notes and footnotes

Footnotes or Notes 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.

Bibliographic reference to the source of statements in the text is made by use of *superior numerals* at the appropriate place. 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). The

references themselves are given at the end of the final printed text along with any Notes.

Authors are encouraged to check the RSC Reviews web site to ensure that they have cited relevant recent reviews.†

4.1 Journals

The style of journal abbreviations to be used in the Society's publications is that defined in Chemical Abstracts Service Source Index (CASSI). The abbreviations listed in CASSI are based upon internationally recognised systems. A list of CASSI-style abbreviations covering the most commonly cited journals is available from our web site.† It is not, of course, a full list; CASSI plus its quarterly supplements run to more than 2000 pages.

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 possible, page number ranges are preferred over single values, but either format is acceptable.

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

Please note that journal citations in articles submitted to the journal *Photochemical & Photobiological Sciences* should include the article titles.

4.2 Books

For example:

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

4.3 Patents

Patents should be indicated in the following form:

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

4.4 Reports and bulletins, etc.

For example:

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.

4.5 Material presented at meetings

For example:

H. C. Freeman, Proceedings of the 21st International Conference on Coordination Chemistry, Toulouse, 1980.

4.6 Theses

For example:

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

4.7 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

A. R. Jones, *Dalton Trans.*, 2003, DOI: 10.1039/paperno.

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.

4.8 Names

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.

4.9 Composite references

Whenever possible, composite references should be used rather than a series of individual references. The style for composite references is as follows:

A. B. Jones, *J. Am. Chem. Soc.*, 1956, **78**, 1234–1246; A. B. Jones and C. D. Brown, *J. Am. Chem. Soc.*, 1957, **79**, 567–569; A. B. Jones and E. F. Green, *J. Am. Chem. Soc.*, 1957, **79**, 999–1048.

Idem, *loc. cit.*, and *op. cit.* are not used in references.