Organic & Biomolecular Chemistry

INDEXED IN MEDLINE

Incorporating Acta Chemica Scandinavica

Instructions for Authors (2004)

Also see www.rsc.org/illustrations and www.rsc.org/electronicfiles

CONTENTS

1.0 General Policy

Organic & Biomolecular Chemistry is a bimonthly journal for the publication of original research papers (articles), communications, Emerging Areas and Perspectives focusing on all aspects of synthetic, physical and biomolecular organic chemistry.

Authors should note that papers that mainly emphasise the novel properties, applications or potential applications of materials may be more suited for submission to *Journal of Materials Chemistry*. (http://www.rsc.org/materials).

There is no page charge for papers published in *Organic & Biomolecular Chemistry*.

Scope of the Journal

Organic & Biomolecular Chemistry brings together molecular design, synthesis, structure, function and reactivity in one journal. It publishes fundamental work on synthetic, physical and biomolecular organic chemistry as well as all organic aspects of: chemical biology, medicinal chemistry, natural product chemistry, supramolecular chemistry, macromolecular chemistry, theoretical chemistry and catalysis.

Contact Details for the Editorial Office

Dr Caroline V Potter, Managing Editor,
Organic & Biomolecular Chemistry,
The Royal Society of Chemistry, The Science Park,
Milton Road, Cambridge, UK CB4 0WF
Tel: +44 (0)1223 432137
Fax: +44 (0) 1223 420247
E-mail: OBC@rsc.org

1.1 Articles

Full papers contain original scientific work that has not been published previously. However, work that has appeared in print in a short form such as an *Organic & Biomolecular Chemistry Communication* or *Chemical Communication* is normally acceptable. But note that the Society strongly discourages the fragmentation of a substantial body of work into a number of short publications.

1.2 Communications

Organic & Biomolecular Chemistry Communications contain novel scientific work of such importance that rapid publication

is desirable. Authors should briefly indicate in a covering letter the reasons why they feel that publication of their work as a *Communication* is justified. The recommended length is between two and five printed journal pages.

1.3 Emerging Areas

Emerging Areas are short, personal accounts of a new area of research. They can be speculative in nature, putting a new area in perspective These are normally published by invitation of the *Organic & Biomolecular Chemistry* Editorial Board. However, suggestions from authors are welcome and enquiries regarding the submission of Emerging Areas should be directed to the Managing Editor.

1.4 Perspective Articles

Perspective Articles are either a concise and critical appraisal or a personal viewpoint of activity in a specialist area of organic chemistry. Perspective articles will be easy-to-read articles covering current areas of interest and not comprehensive reviews of the literature. These are normally published by invitation of the *Organic & Biomolecular Chemistry* Editorial Board. However, suggestions from authors are welcome and enquiries regarding the submission of Perspective Articles should be directed to the Managing Editor.

1.5 Submission of Articles

Authors should send submissions to the Journal in electronic form using the RSC e-submission service (www.rsc.org/submissions).

On submitting their manuscripts, authors are encouraged to supply the names and addresses of 2–3 potential referees. For an *Organic & Biomolecular Chemistry Communication* authors should briefly indicate in a covering note or letter the reasons why they feel that rapid publication of their work is justified. Authors should highlight the novel aspects of the organic or biomolecular chemistry within the paper.

All authors submitting work for publication are required to sign an exclusive copyright license. This License to Publish should be agreed during the submission process or alternatively a form may be forwarded to the Editor by fax or post (www.rsc.org/is/journals/current/coplic.htm).

Rapid publication is aided by careful preparation of text and illustrations. Particular attention is drawn to the use of (*i*) SI units and associated conventions, (*ii*) IUPAC nomenclature for compounds and (*iii*) standard methods of literature citation.

1.5.1 E-submissions. Articles should be submitted to the Editorial Office using the RSC file-upload service: http://www.rsc.org/submissions

The RSC e-submission service allows any number of files to be uploaded to the Cambridge *Organic & Biomolecular Chemistry* Offices. The following files and information should be provided:

(a) The manuscript as a single Word file or PDF with figures embedded. This file will be used for online refereeing where possible.

(b) Crystallographic data in CIF format (if appropriate, see Section 5.0).

(c) Data for deposition with the ESI service (if appropriate, see Section 3.4).

(d) Details of any relevant preliminary Communications (please give reference or include PDF file).

(e) Names of potential referees.

(f) A justification of why the work merits urgent publication if the submission is a Communication.

(g) A Licence to Publish should be agreed during the submission process or alternatively a form may be forwarded to the Editor by fax or post (www.rsc.org/is/journals/current/coplic.htm).

After e-submission your file will be acknowledged by the Editorial Office as soon as possible. Authors should contact the Editorial Office if they have not received an acknowledgement within 4 working days.

For manuscripts submitted online a printed copy of the manuscript will **not** be required.

1.5.2 North American Office. Authors from the USA and Canada may address their manuscripts to:

Professor Peter Wipf, Associate Editor for North America,
Organic & Biomolecular Chemistry
Department of Chemistry, University of Pittsburgh
Pittsburgh, PA 15260, USA
Tel: +1 412 624 8606
E-mail: pwipf+@pitt.edu

1.5.3 Requirements for Revised Articles and Material for Proof Preparation. Revised manuscripts may be sent to the Editorial Office either by electronic file upload (http://www.rsc.org/submissions) or by post to the addresses above. Revised manuscripts sent by post can be accepted on 3.5 inch disk, ZIP disk or CD-ROM and should be accompanied by a printed copy of the manuscript. Please ensure that the electronic version is identical with the hardcopy.

Please note that when an article is accepted for publication, a MS Word (or similar native format) version of the manuscript and separate copies of the artwork in TIFF, EPS or PDF formats will be required at that time for proof preparation. Unfortunately PDF files and MS Word files containing encapsulated figures are **not** suitable for proof preparation.

Further details on revised file formats are given in the separate Guidelines on submitting files for proof preparation given in Section 3.5.

2.0 Administration

Receipt of a paper will be acknowledged, and the paper will be given a reference number which authors are asked to quote on all their subsequent correspondence. If no such acknowledgement has been received after a reasonable period of time, authors should check with the Editorial Office as to whether the paper or the acknowledgement has gone astray.

Editorial Policy. All manuscripts will be processed in an efficient, fair and timely manner. Papers that are accepted must not be published elsewhere except by permission of the Royal Society of Chemistry. Submission of a manuscript will be regarded as an undertaking that the same material is not being considered for publication by another journal. Conditions governing acceptance are available from the Editorial Office. Full details are given in *Refereeing Procedure and Policy* at http://www.rsc.org/pdf/authrefs/ref.pdf and in *Ethical Guidelines* http://www.rsc.org/pdf/journals/ethicalguidelines.pdf

Copyright. The whole of the literary matter (including tables, figures, diagrams and photographs) in *Organic & Biomolecular Chemistry* is subject to copyright and may not be reproduced without permission from The Royal Society of Chemistry and such other owner of the copyright as may be indicated. However, the owner may reproduce/republish portions of the Work without seeking permission, provided any reproduction is accompanied by an acknowledgement in the form:

(original citation) – Reproduced by permission of the Royal Society of Chemistry.

To republish/reproduce the whole Work, the copyright Owner must submit a written request to the RSC. The RSC will agree to any reasonable request, provided that the owner ensures that any such replication is accompanied by an acknowledgement (in the above form) of first publication of the Work by the RSC.

Reprints. A PDF reprint of each paper will be supplied free of charge.

3.0 Notes on the Preparation of Papers

3.1 Organisation of Material

(a) Authors may prepare manuscripts on the RSC template, available at www.rsc.org/is/journals/templates/templates.htm, however this is not a requirement.

(b) Pages should be numbered sequentially.

(c) The first page should be set out as follows:

(i) Name and address of the author to whom the proofs and correspondence should be sent.

(ii) Title of the paper, with a capital initial letter only.

(iii) The use of Series titles and Part numbers in titles of papers is not permitted. 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.

(iv) Authors' names, including one forename for each author; an asterisk should follow the name of the author who is to receive correspondence. An e-mail address may be included at the end of the address of the author who is to receive correspondence.

(v) The address where the work was carried out; if this is different from the current address of any author wishing to deal with correspondence, a footnote indicating the present address of this author should be included. For multiple authors at different locations italic superior letters (*a*,*b*,*c* . . . following the asterisk if present) should be used to identify addresses.

(vi) Abstract, followed by a horizontal line, in double-line spacing.

(d) The article should be set out in the following order:

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

(ii) 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.

(iii) 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 and expected hazards encountered during the experimental work should be noted. In general there is no need to report unsuccessful experiments.

(e) Bibliographic references, or References and Notes, should be numbered serially in the text by means of superscript arabic numerals.

(f) Notes and References should follow the main text and should have the following format:

1 A. Smith, *Org. Biomol. Chem.*, 2003, **1**, 2973–2980

2 A. J. L. Beckwith and K. U Ingold, in *Rearrangements in Ground and Excited States*, ed. P. de Mayo, Academic Press, New York, 1980, vol. 1, p. 161.

3 The more commonly used reduced temperature scale (T/T_{NI} in K) gives similar results.

Page ranges are preferred, however both formats are acceptable.

(g) Journal titles should be abbreviated according to the Chemical Abstracts Service Source Index (CASSI).

(h) **Reviews web site**: Authors are encouraged to check our Reviews web site to ensure that they have cited relevant recent reviews: www.rsc.org/reviews

(i) A graphical contents entry should be provided with each submission. This should include: Graphic: 8 cm × 4 cm **preferably in colour**. Text: one sentence no longer than 20 words, highlighting the most interesting and novel parts of the manuscript. The text provided may be rewritten to maintain the journal style.

(j) 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. Titles, Mr, Mrs, Miss, Ms, Dr, Professor, *etc.*, should be given but not degrees.

(k) 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 in 5 year intervals) and *in memoriam* dedications would be considered appropriate. Other forms of dedication may require approval of the Editorial Board.

(l) Tables should be prepared on separate pages at the end of the manuscript.

(m) Diagrams should be provided on separate pages at the end of the manuscript and accompanied by a separately typed set of captions. Text and diagrams should not be combined.

(n) Revised manuscripts should be submitted in electronic form and be accompanied by a hard copy only if sent by post. The Guidelines for submission of files for proof preparation are given in Section 3.5.

(o) *Communications* should include brief details of key experiments (with amounts of reagents used) but more extensive supporting data are not required; these can be provided as supplementary information to assist referees in their assessment of the work.

3.2 Artwork Guidelines

All formulae and figures should be clear and, in the case of figures, provided with captions on a separate page. Illustrations should be prepared for a single (83 mm) or double column (171 mm) width. Single column is preferred and the maximum page depth is 258 mm. Artwork sent by post should be supplied at its *final* size so that reduction is not required. The best copy originals or electronic files should be supplied as photocopies are rarely suitable for reproduction.

3.2.1 Line illustrations. (a) Line illustrations should be drawn in black, using lines of an even and adequate thickness (*e.g.* 1 pt). Curves should be smooth. Broken, dotted and dot-dash lines may also be used. Particular care should be taken to ensure that lines in spectra are of an adequate thickness (*i.e.* not less than 1 pt) for reproduction.

(b) Experimental data points must be of a reasonable size and wherever possible confined to open and closed circles, crosses, squares and triangles. Partly black circles and similar signs frequently become indistinguishable in print.

(c) Avoid the use of shading (tints) that simulate grey and use line shading if appropriate. Diagrams containing several grey shades are unlikely to reproduce successfully.

(d) If possible, lettering should be in an 8 pt Helvetica/Arial font.

(e) For graphs, axis labels should use SI units, separated from quantities with a solidus '/' *not* brackets, *e.g.* λ/nm, $10^3(T/\mathrm{K})^{-1}$, 2θ/degrees. Symbols representing physical quantities should be

given in italics, *e.g.* *t*/s, and units should be expressed in the form, *e.g.*, g ml^{-1} rather than g/ml. Please note that % and ppm are ratios rather than units and should therefore be given in brackets.

(f) Extensive identifying lettering should be placed in the captions, rather than on the figures. Curves may be referred to by (*a*), (*b*), (*c*) *etc*. on the figure.

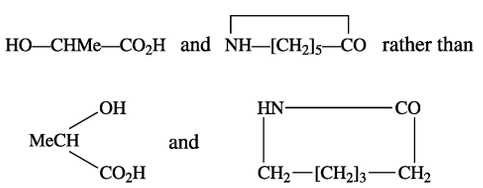
3.2.2 Structural Formulae. The purpose of all illustrative matter in a paper is to clarify the arguments and descriptions rather than to duplicate them. The RSC strongly encourages the use of displayed formulae, particularly in the form of schemes where the details of a reaction sequence are often more easily understood when illustrated than when described in the text.

Advice on the preparation of artwork is available from the Editorial Office.

(a) Formulae should be numbered with bold arabic numerals, **1**, **2** and **3** *etc*.

(b) In complex reaction schemes formulae should preferably be numbered serially following the reaction sequence. Non-sequential numbering in a collection of formulae can render it difficult to locate an individual number.

(c) Formulae inserted into the body of the text (as distinct from those displayed separately) should be written on one line, *e.g.*



(d) Steric conventions should be observed, notably for steroids, triterpenes and carbohydrates. The RSC prefers wedges (▲) or heavy lines (—) rather than blocked circles (●), and dashed lines in the form – – – –.

(e) The key number for a compound may be used in the cursive text to avoid repetition of long chemical names. In general it is preferred if the key number is qualified by a partial name.

(f) Reference to compounds in the summary by key number alone is discouraged, since a summary should be comprehensible without reference to the body of the paper.

(g) Structures and schemes can be submitted electronically. The settings for ChemDraw 3.5 are: *Drawing settings*: chain angle 120° bond spacing 20% of length; fixed length 0.43 cm; bold width 0.056 cm; line width 0.016 cm, margin width 0.044 cm, hash spacing 0.062 cm. *Text settings*: font labels and atom labels should be in 7 pt Helvetica/Arial; fractional character widths should be enabled. ChemWindow files should be saved as <*filename*>.cwg, ISIS/Draw saved as <*filename*>.skc and Chemsketch saved as <*filename*>.sk2.

(h) To facilitate rapid processing of your work and to avoid omissions please ensure that submitted manuscripts clearly indicate the desired location of unnumbered graphics in the text, *e.g.* **<structures 1 to 3 here>**.

3.2.3 Colour. The use of colour is freely available to all authors.

(a) Avoid tints or shading and if possible use only the following colours (other colours may not reproduce well);

100% magenta

100% cyan

100% magenta + 100% process yellow (to give red)

100% cyan + 100% process yellow (to give green)

(b) Reproduction of colour figures is best from computer generated artwork which should be saved as .TIF or .EPS files at ⩾300 dpi resolution, 600 dpi is preferred.

(c) Good quality hard copies from a high-resolution printer may be supplied (preferably from a professional bureau). Inkjet printers are unlikely to give output of sufficient quality.

3.3 Nomenclature

Current IUPAC nomenclature and symbolism should be used. Attention is drawn to the following publications in which the rules themselves and guidance on their use are given:

Nomenclature of Inorganic Chemistry, Blackwell Scientific Publications, Oxford, 1990.

Nomenclature of Organic Chemistry, Pergamon, Oxford, 1979 edn.

A Guide to IUPAC Nomenclature of Organic Compounds, Blackwell Scientific Publications, Oxford, 1993.

Biochemical Nomenclature and Related Documents, Portland Press, London, 1992.

Compendium of Chemical Terminology: *IUPAC Recommendations*, Blackwell Scientific Publications, Oxford, 1997.

Guidelines for macromolecular nomenclature are now available on the World Wide Web at:

http://www.iupac.org/publications/books/author/metanomski.html

http://www.iupac.org/reports/IV/guide.html

Units and Symbols

The recommendations of IUPAC should be followed. Their basis is the Système Internationale d'Unités (SI). A detailed treatment is given in the so-called Green Book: *Quantities, Units and Symbols in Physical Chemistry*, Blackwell Scientific Publications, Oxford, 1993 edn.

3.4 Deposition of Supplementary Data

Information (such as spectra, primary kinetic data, computer programs, and output, evidence for amino acid sequences, *etc*.), which accompanies papers may be deposited, free of charge, with the Society's Electronic Supplementary Information service (ESI), either at the request of the author and with the approval of the referees or on the recommendation of referees and with the approval of the author. In cases where repetition occurs in the experimental section, only key procedures should be presented in the paper with the remainder, where possible, transferred to ESI.

Under this scheme, authors should submit articles and the supplementary material to the *Journal* simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication, electronic supplementary material will be mounted on the RSC web server in an appropriate file format. The supplementary material will be available from the RSC web site at the internet address that will appear in the article.

3.4.1 Preparation and Submission of Material. Authors will be responsible for the preparation of the supplementary material. Electronic material should be supplied where possible in the following file types:

(a) Microsoft Word

(b) WordPerfect

(c) Crystallographic Information File (CIF)

(d) XYZ, MDL MOLFile (MOL) or Brookhaven Protein Databank (PDB) files

(e) JPEG/GIF (maximum size 640 × 480 pixels)

Authors must identify which manuscript the electronic file is associated with when they send the file to the Editorial Office by entering the name of the manuscript at the top of the electronic file. CIF files should be sent by e-mail or supplied as part of the file upload, according to the instructions in Section 5.3.

3.4.2 Availability. Electronic supplementary information may be accessed free of charge from the RSC web site (http://

www.rsc.org/esi) and for those without web access copies may also be obtained from the RSC Library and Information Service:

Library and Information Centre, The Royal Society of Chemistry, Burlington House, Piccadilly, London, UK W1V 0BN, Fax: 0171 287 9798, e-mail: Library@rsc.org

3.5 Guidelines on submitting files for proof preparation

Successful use of your electronic files should speed up the production process and avoid errors being introduced.

3.5.1 Uploaded Files. (a) The electronic files for proof preparation (for formats see below) should be for the revised version of the manuscript. At this stage do not provide PDF files.

(b) Please supply the manuscript text (incorporating any revisions) and the graphics (for formats see below) as separate files, since these have to go through different production stages.

3.5.2 File Types. (a) We prefer to receive Microsoft Word files, although we will endeavour to use other electronic versions wherever possible. For other word processors, also save the file as Rich Text Format (*.rtf*) if possible.

(b) *Graphics*. ChemDraw files (saved as *filename.cdx*) are preferred, but we can also accept ChemWindows (saved as *filename.cwg*), Isis/Draw (saved as *filename.skc*) and ChemSketch (saved as *filename.sk2*).

(c) Please do not integrate your graphics files into the word processor document, since these are difficult to separate out for the proof preparation process.

3.5.3 Tables. Please include any tables at the end of the text file, and use either the word processor's table editor or tabs for formatting (but not a mixture of the two).

3.5.4 Graphics. (a) **Chemical structures** as ChemDraw, ChemWindows ChemSketch and ISIS/Draw files submitted separately to the manuscript.

(b) **Artwork** (other than structures) as TIFF, EPS or PDF at 600 dpi or greater resolution. It would be helpful if PDF graphics were produced using the "PDF Creation Files" job options from our web site: http://www.rsc.org/is/journals/templates/templates.htm

(c) Please supply these separately to the word-processed file.

3.5.5 Consistency. Check the manuscript carefully for consistency, particularly in the representation of chemical formulae, compound names and words with alternative spellings.

We will try to use the supplied data in our production process, but mathematical equations and tables, in particular, may be rekeyed by the typesetter. Page proofs should still be checked closely.

4.0 Experimental and Characterisation Requirements

4.1 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.

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%).

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.

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

Refractive index. Given in the form $n^{22}{}_D$ 1.653.

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].

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.

IR absorptions. Shown 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).

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.

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).

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).

Example of a typical experimental section format. The following paragraph exemplifies many of the points made in the preceding paragraphs.

(*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 × 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. $C_{11}H_{20}O_2$ requires C, 71.7; H, 10.9%); ν_{max}(film)/cm^{-1} 3342, 1777, 1711, 968 and 766; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.45 (2 H, quintet, *J* 7.4, $CH_2CH_2CH_2$), 1.65 (2 H, br s, OH), 2.03 (4 H, dt, *J* 6.6 and 7.4, 2 × CH_2CH=CH), 2.27 (4 H, dt, *J* 7.6 and 6.3, 2 × CH_2CH=CH), 3.63 (4 H, t, *J* 6.3, 2 × CH_2OH) and 5.34–5.61 (4 H, m, 2 × CHCH); δ_C(67.8 MHz; $CDCl_3$; Me_4Si) 29.3 (t), 32.3 (2 × t), 36.2 (2 × t), 62.3 (2 × t), 126.6 (2 × d) and 133.4 (2 × d); *m*/*z* (EI) 154.1334 ($M^+ - CH_2O$. $C_{10}H_{18}O$ requires 154.1358), 135 (7%), 125 (7), 107 (24), 98 (38) and 81 (100).

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

4.2 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 3.4) 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.

4.3 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%.

5.0 Small Molecule Single Crystal X-Ray Crystallographic Data

Crystallographic work will be assessed for its chemical interest. Thus crystallographic work carried out as part of a wider chemical study should not normally be submitted separately from the results of that study.

The description of a crystallographic structure determination should be as brief as possible, consistent with the following guidelines, and should be included at the end of the paper (or at the end of the Experimental section, if this precedes the Discussion). An expanded version of instructions for publication of crystallographic work can be found on the RSC web site (http://www.rsc.org/is/journals/authrefs/cryst.htm).

5.1 Title and Summary

For a paper reporting a crystallographic structure determination it is often appropriate, although not essential to indicate this information in the title, *e.g.* by the words 'crystal structure of'. For papers which contain several crystal structure determinations it is recommended that lengthy titles quoting the formula of all the structures determined be avoided. Whether or not the crystal structure determination is indicated in the title, reference should be made to it in the summary. The summary need not contain cell dimensions and other crystal data.

5.2 Presentation of Crystal Data in the Manuscript

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. For purely inorganic compounds a table of atomic coordinates may also be included.

5.2.1 For Full Papers. 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 (for example it is rarely necessary to include data for phenyl rings). Average values may be given (with a range of e.s.d.s) for chemically equivalent groups or for similar bonds. Differences from expected norms should be noted.

5.2.2 For Communications. Details of the data collection and structure analysis should be given in a footnote or in the References/Notes section (see Section 4.2.4). Selected bond lengths and angles, with estimated standard deviations, should

be included in the figure captions and be restricted to significant dimensions only.

5.2.3 Illustrations. 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. Any differences from that required by standard rules of chemical nomenclature should be pointed out. Each atom of the asymmetric unit should be assigned an arabic numeral in parentheses following the chemical symbol: C(2), O(1''), *etc*.; it is often convenient to associate a particular number of primes with a particular asymmetric unit. Alternatively, roman numeral superscripts can be employed: $C(2^{I}) \cdots C(2^{IV})$.

Where CIF files are available, authors are encouraged to enhance their papers by converting the crystallographic data into XYZ, MOL or PDB formats. These files give a 3D representation of the structure which can be viewed and manipulated on screen using the free internet browser plug-in CHIME. The files would be made available free of charge as electronic supplementary information (ESI). For further details and an online tutorial, see http://www.rsc.org/is/journals/authrefs/3DFigures.htm

5.2.4 Data Required for Presentation in the Manuscript. For both full papers or communications, the following information should be given in the manuscript:

(1) Chemical formula and formula weight (M)
(2) Crystal system
(3) Unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, temperature
(4) Space group symbol (if non-standard setting give related standard setting)
(5) No. of formula units in unit cell (Z)
(6) Linear absorption coefficient (μ)
(7) Number of reflections measured and/or number of independent reflections and R_{int}
(8) Final R values (and whether quoted for all or observed data)

The following example demonstrates the application of the recommendations for a full paper. For a communication, the headings should be omitted and the text placed in a footnote or the References/Notes section.

Experimental

Single crystals of compound **2** suitable for X-ray diffraction were selected directly from the analytical samples.

Crystal structure determination of compound 2

Crystal data. $C_{58.5}H_{62}N_4O_{8.5}$, $M = 957.12$, orthorhombic, $a = 25.7972(4)$, $b = 16.5089(3)$, $c = 23.7612(4)$ Å, $U = 10119.5(3)$ Å^3, $T = 150(1)$ K, space group *Pbcn* (no. 19), $Z = 8$, μ(Mo-Kα = 1.9 mm^{-1}, 69128 reflections measured, 10286 unique ($R_{int} = 0.031$) which were used in all calculations. The final $wR(F^2)$ was 0.1312 (all data).

5.3 Supplementary Data Required for Assessment and/or Deposition

Authors should submit all supplementary crystallographic data as a Crystallographic Information File (CIF) file either *via* electronic mail to OBC@rsc.org or as part of the e-submission (see Section 1.4.1). Authors should combine multiple data sets for a given manuscript into a single file. This will minimise the chance that files will be misplaced or associated with the wrong manuscript. 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 send the file to the Editorial Office by entering the name of the manuscript at the top of the electronic file. The information required for deposition includes:

(1) A table of final fractional atomic coordinates.
(2) Any calculated coordinates (*e.g*. hydrogen)
(3) A full list of bond lengths and angles with estimated standard deviations.
(4) A full list of displacement parameters in the form B_{ij} or U_{ij} (in Å^2 or pm^2)
(5) FULL details of the refinement.

A full checklist of data items required for deposition, together with full details for CIF submissions, are available by request from the editorial office or *via* the World Wide Web (http://www.rsc.org/is/journals/authrefs/cryst.htm).

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. If the data are not available in electronic form then two hard copies of items 1–5 above should be included with the paper at the time of submission.

5.3.1 Deposition of Material at the Cambridge Crystallographic Data Centre. 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 metallo-organic compounds will be entered into the Cambridge Structural Database. Post-publication requests for individual data sets (organic or inorganic) should be directed to CCDC, 12 Union Road, Cambridge, UK CB2 1EZ (e-mail: deposit@ccdc.cam.ac.uk, Fax: +44 (0)1223 336033).

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.

5.4 Reference to Crystallographic Work Published in a Preliminary Communication

It is permissible to regard a fully refined crystal structure determination published in a *Communication* as archival material. If an author does not wish to discuss the structure again at any length in the corresponding full paper, this purpose will be served by a simple reference back to the original communication, and need not be re-presented for publication or for the referees. However if these conditions are not fulfilled, the data should be re-presented *in full* and will be re-published if considered necessary.

5.5 Reference to Unpublished Crystallographic Work

There may be cases (other than that just described) 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. He/she may not even wish to include the crystallographer as co-author (for example when the determination is carried out by a commercial company). If the author is able to show that this procedure is appropriate, it will be allowed provided that it does not lead to unnecessary fragmentation. However the author must provide, as supplementary information, sufficient data relating to the crystal structure determination to allow a crystallographer to make sure that the point made is correct, and coordinates *etc*.

will be deposited at the Cambridge Crystallographic Data Centre. The brief published description of the determination should be supplemented by appropriate reference to 'unpublished work'.

6.0 Macromolecular Structure Determination and Sequence Data

6.1 Novel macromolecular structures

All manuscripts that report novel macromolecular three-dimensional structures at the level of individual atomic positions must be accompanied by deposition of the required structural data in the appropriate database (usually PDB or NDB—see contact details below) to support the conclusions drawn. 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. For X-ray structures, PDB header information (*i.e.* R_{merge}, completeness, multiplicity and $I/\sigma I$ (both overall and in the outer resolution shell) for data, and R_{cryst}, R_{free} 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 in as summary data tables in the manuscript, or as ESI.

Deposited files must be released immediately on publication. A six-month delay will be considered only in exceptional circumstances. Articles will not be published until the relevant PDB or NDB 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.

6.2 Sequence data

Newly reported nucleic acid or protein sequences must be deposited with the appropriate database: EMBL, GenBank, DDBJ, SWISS-PROT or PSD (see below for contact details). Deposited files must be released immediately on publication of the article, which will not be published until an accession number is quoted in the experimental section of the manuscript and the abstract.

Contact details for structure and sequence databases

Protein Data Bank
http://pdb.rutgers.edu
deposit@rcsb.rutgers.edu
or
http://www.ebi.ac.uk/msd/
pdbhelp@ebi.ac.uk

Nucleic Acids Database
http://ndbserver.rutgers.edu
ndbadmin@ndbserver.rutgers.edu

EMBL Nucleotide Sequence Submissions
http://www.ebi.ac.uk/Submissions/
datasubs@ebi.ac.uk

National Center for Biotechnology Information (GenBank)
http://www.ncbi.nlm.nih.gov
info@ncbi.nlm.nih.gov

DNA Data Bank of Japan
http://www.ddbj.nig.ac.jp
ddbj@ddbj.nig.ac.jp

SWISS-PROT submissions
http://www.ebi.ac.uk
datasubs@ebi.ac.uk

Protein Information Resource (Protein Sequence Database, PSD)
http://www-nbrf.georgetown.edu/pir/
pirmail@nbrf.georgetown.edu

7.0 Publication of Theoretical and Computational Papers

Authors should note the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

(i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to *PCCP*, one in which the computations are applied to the chemistry/biology to *Organic & Biomolecular Chemistry*, *Dalton*, or *PCCP*. Papers concerned mainly with computational details are unlikely to be accepted for Organic & Biomolecular Chemistry.

(ii) The purpose of the paper and the precise objectives of the calculations performed should be clearly stated; the results obtained should be reported only in so far as they relate to those objectives.

(iii) Many papers use a routine procedure based on a well documented method, be it semiempirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer program used and to indicate briefly any modification made by the author. A review of theoretical background would be out of place, but an author should say why she/he considers the method adequate for her/his purposes.

(iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited as supplementary data (see Section 3.4). Such material should be submitted with the main paper, clearly distinguished from it, and referred to as a footnote to the title.

8.0 Molecular Modelling Guidelines

Molecular modelling studies should be subject to the same rigorous scientific standard required of other types of experiment, such that objective evaluation by independent investigators is possible. Authors are therefore strongly encouraged to provide sufficient details of any computationally assisted modelling results they report that might assist in any such evaluation. This information should include:

(a) A precise description of any computer software used, including any version or revision numbers, the type of computer used and a reference to a source for the program or a published definition of the algorithm used.

(b) A concise indication in a Computational Details section or a footnote of standard options involved such as basis sets, SCF methods, electronic states, parameter sets, charge distribution schemes, symmetry, geometry optimization methods, convergence criteria, cut-offs, time constants, *etc*. More explicit details of any non-standard use of *e.g*. basis sets,

force-field parameters and algorithmic options, should be particularly provided.

(c) Key stationary points in a potential surface which are essential to conclusions discussed in the text should be accurately characterized by reporting *e.g*. the calculated energy and important geometrical parameters. Authors are encouraged to provide more complete information such as atom types, molecular coordinates and connectivity data if available for these points in the form of supplemental tables, or preferably in computer-readable form as *e.g*. program input data sets or archive files.

Further details of proposed guidelines in molecular modelling are to be found in P. Gund, D. C. Barry, J. M. Blaney and N. C. Cohen, *J. Med. Chem.*, 1988, **31**, 2230.

9.0 Natural Product Structure Elucidation Papers

Natural product structure elucidation papers will be accepted for publication in the *Organic & Biomolecular Chemistry* only if they are of sufficient novelty and interest or if the structure described is of intrinsic interest; in this context, intrinsic interest is defined as having skeletal or constitutional novelty. Manuscripts describing the structural elucidation, by routine methods, of compounds which are similar to known compounds and which display no interesting or unusual properties would not normally fulfil these criteria.

10.0 Animal Welfare

In cases where an experiment involves the use of live animal, the Methods section of the manuscript should include a statement that all experiments were performed in compliance with the relevant laws and institutional guidelines, and should identify the institutional committees that have approved the experiments where applicable. Referees may be asked to comment specifically on any cases in which concerns may arise.