Notice to Authors, 1992

Refereeing Policy

Chemical Communications provides a forum for preliminary accounts of original and significant work that is likely to prove to be of wide general appeal or exceptional specialist interest. Such reports should eventually be followed up by full papers providing detailed accounts in other journals.

The policy of the Society remains that only a fraction of research work warrants publication in *Chemical Communications*, and strict refereeing standards will, therefore, apply. The benefit to the reader from the rapid publication of a particular piece of work before it appears as a full paper must be balanced against the general desirability of avoiding duplicate publication. The needs of the reader, not the author, must be considered, and priority in publication is not a factor in determining acceptability. Contributions are accepted by the Society on the understanding that authors will not have submitted the same material for publication elsewhere during its consideration by the Society.

Authors should briefly indicate in a covering note or letter (two copies) the reasons why they feel that publication of their work in *Chemical Communications* is justified. Each communication is assessed by two independent referees and a further referee if their recommendations differ. Firm concurring recommendations from two referees are required for acceptance or rejection. Authors of refused communications will have the right to appeal, through the Editor, to Journals Management Committee. Short articles that have the detail of content and argument appropriate to the definitive paper but do not meet the criteria in paragraph one should be submitted to the appropriate section of *J. Chem. Soc., Dalton, Perkin,* or *Faraday Trans.*, or to *J. Chem. Research* or *J. Mater. Chem.*

As noted above, it is necessary in most cases to publish a full paper as a follow-up to the preliminary communication. However, authors should note that the acceptance of a contribution to *Chemical Communications* does not guarantee that the accompanying full paper will be acceptable for one of the Society's journals.

Administration

An acknowledgement of receipt will be sent by first-class mail or airmail to the author submitting a manuscript. Authors should contact the editorial office if an acknowledgement is not received within a reasonable time. Authors will be informed of the referees' recommendation as soon as concurring reports have been obtained. The editorial staff will do their best to ensure that communications are refereed promptly, but delays may sometimes occur, particularly during holiday periods.

The editorial office may be contacted by any of the means given on the inside front cover of each issue. When appropriate, the editorial staff will use fax or electronic mail for correspondence. **Authors should include their fax number** (and if possible their **electronic-mail address**) in their letter of submission. They should tell the editorial staff whether they would like the referees' comments to be sent by fax or E-mail.

Authors should respond to referees' recommendations and return proofs without delay, or let the editorial staff know immediately if their response is likely to be delayed. Failure to respond to referees' comments, or to return proofs, within one month of the date of despatch may lead to the communication being regarded as withdrawn.

Manuscripts.—*General.* Individual articles should be as brief as possible, and should be restricted to the central urgent theme; they should not normally exceed approximately $1–1\frac{1}{2}$ printed pages in length. Extensive historical introduction, experimental detail, physical data and mechanistic conjecture will, in general, not be published; however, authors are strongly encouraged to include supplementary information that they feel will aid the referees in their assessment of the work. Illustrations and tables will only be published if necessary for ease of comprehension by the reader. For work involving microorganisms, sufficient detail should be given to identify the species being used.

Presentation. Careful attention to the following points will aid rapid publication.

(a) **Four** copies of the manuscript must be provided. One should be a top-quality original, in double-line spacing, typed on one side of the sheet only. Margins of at least 4 cm must be left at the top, bottom, and left-hand side.

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

(i) Title, capitals for the first letter of each noun and adjective only.
Note: The inclusion of 'Series or Part numbers' in the title of a communication is not allowed.

(ii) Authors' names, with one forename for each author. The author to whom subsequent correspondence arising from publication of the communication should be addressed may be indicated by an asterisk (*) by the name. For indexing purposes, authors should indicate that part of their name to be used as their surname if there is any possibility of ambiguity.

(iii) Authors' address.

(iv) An extra line of space.

(v) A one-sentence summary.

(vi) An extra line of space.

(vii) Main text, first paragraph not indented.

(c) Spacings must be those required in print, *e.g.* each paragraph must be indented. A space must be left after numerals (except where these occur in chemical names), when these qualify units (*e.g.* 3 g), but not when they are multiples (10^3k).

(d) Attention should be paid to underlining, and punctuation (or its absence) in symbols and chemical names. Greek letters and special symbols should be explained by marginal notes (*e.g.* Gk nu) the first time that they appear and should not be underlined.

(e) Alterations must be made by complete erasure, or by crossing out the error and writing the correct version above it.

(f) Bibliographic references are indicated in the text by superior numerals and must be cited in numerical sequence. The bibliography should include the authors' initials given before the surnames and should be set out on a separate sheet. Textual footnotes should be presented separately from the numbered bibliography, and given symbols in the sequence †‡§¶‖.

(g) Captions to illustrations should be presented on a separate sheet and be clearly labelled.

Illustrations.—*General.* Structural or displayed formulae must be carefully and accurately drawn or typed on a separate sheet, rather than inserted into the text; numbered formulae must be displayed in numerical sequence.

Submission of Structure Diagrams on Disk. The Society is willing to receive ChemDraw-produced structure diagrams, reaction schemes, *etc.*, on disk, provided that the data files are supplied in the appropriate format. To facilitate this, the Society will provide, on request, a 3.5″ Macintosh diskette containing the preference files and column guides appropriate for producing suitable output with ChemDraw version 2.1.3. Authors wishing to take advantage of this arrangement will be advised to copy these files to their own storage media (diskette or hard disk) for future use. No guarantee can be given that structures produced in this way will be used as submitted, but it is expected that this route will minimise duplication of the efforts of authors and production staff. To obtain a copy of the diskette, contact Alan McNaught (Manager, Journals) at the Society's Cambridge office. The page set-up for preparation of drawings and printing should be 60%. Single column (8.3 × 22.8 cm) layout is preferred, for flexibility; however, double column (17.1 × 22.8 cm) is acceptable. The preference settings to be used are as given below.

Other Illustrations. These should be good-quality Indian ink drawings suitable for reduction to about 6 cm in width and drawn with lines of appropriate thickness. Lettering should be clearly but lightly inserted in pencil.

The Title

The title should clearly and accurately indicate the content of the communication and be expressed in scientific terms that can function as 'points of entry' for retrieval purposes. Brevity in the title, though desirable, should be balanced against accuracy and usefulness.

The Summary

The summary should be a one-sentence account of the discovery being announced. It must clearly indicate the content that makes the communication important or urgent and be informative rather than indicative, *i.e.* be of the form: 'Reaction of sodium with ethanol in dry benzene gives the monomeric sodium ethoxide' and not 'The reaction of sodium with ethanol in dry benzene has been studied.'

Nomenclature

For many years the Society has actively encouraged the use of standard IUPAC nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Attention is drawn to the following publications in which both the rules themselves and guidance as to their use are given.
Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, 1979 edn., Pergamon, Oxford.
Nomenclature of Inorganic Chemistry, 3rd edn., Blackwell Scientific Publications, Oxford, 1989.
Quantities, Units and Symbols in Physical Chemistry, Blackwell Scientific Publications, Oxford, 1988.
Biochemical Nomenclature and Related Documents, Portland Press, 1992.

A complete listing of all IUPAC nomenclature publications appears in the Instructions for Authors (Appendix), in Issue No. 1 each year of *J. Chem. Soc., Dalton* or *Perkin Trans.* If there are no IUPAC rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff.

Acknowledgements

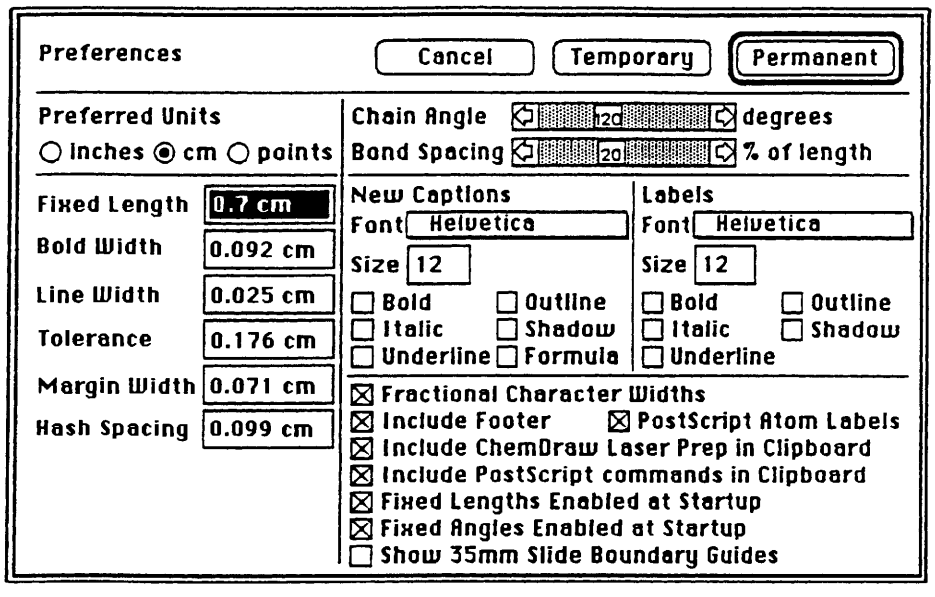
Only personal acknowledgements and those indicating financial support of the research will be published.

Proofs

Proofs will normally be sent by first-class mail—by airmail when appropriate—to the person submitting the article or to the person designated by him or her.

Reprints

Reprints will be printed in the form of a four-page folded sheet, with the title and reference repeated on the front page. An order form for reprints will be supplied with the proofs, and this should be returned as soon as possible, preferably with the corrected proofs. Fifty reprints may be ordered free of charge, and additional reprints may be purchased.



ChemDraw preferences screen

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 an 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 optimisation methods, convergence criteria, cut-offs, time constants, *etc.* More explicit details of any non-standard use of *e.g.* basis sets, force-field parameters, algorithmic options, *etc.* should be provided.

(c) Key stationary points in a potential surface which are essential to conclusions discussed in the text should be accurately characterised 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.

Crystallographic Articles

(a) Crystallographic papers are of two types:

(A) The majority, which contain definitive data on completely refined determinations.
(B) A minority, which include brief accounts of structures containing feature(s) of unusual interest and where the structure solutions are clear but where (for any of a variety of reasons) the full refinement has not been completed. These are then regarded as preliminary publications, at least so far as the X-ray results are concerned.
Both types of publication are appropriate for *Chemical Communications.*

(b) Communications will often contain the information in their titles that an X-ray structure determination has been carried out; however this is not obligatory, especially if the X-ray determination forms only a minor part. Summaries should always contain this information unless the communication is of type (B), and the structure determination is not a main point.

(c) For communications of both types (A) and (B) authors should submit as supplementary information, with the manuscript, tables of atomic coordinates, bond lengths and angles (with standard deviations), thermal parameters (in the form U_{ij} with units of Å^2 or defined by a given formula), observed and calculated structure factors, and full experimental details for the determination. If the communication is accepted, this material (except structure factor tables and experimental details) will be deposited at the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ (or at the Institut für Anorganische Chemie, Universität, Gerhard-Domagk-Str. 1, D-5300 Bonn, *via* Prof Dr G. Bergerhoff, for molecules not containing 'organic' carbon). All tables should be of publicable quality. Computer printout is acceptable provided that it is clearly legible. The print program used should yield concise tables of atomic and other derived parameters. The content of the tables should be non-redundant, and their interpretation immediately obvious. The thermal parameters should be submitted as separate tables, with clear definition of the units used. Any request to Cambridge or to Bonn for data should be accompanied by the full literature citation for the communication concerned.

(d) On occasions *Chemical Communications* will publish preliminary accounts [type (B)] of crystal structures of unusual *chemical* interest. By 'preliminary' is meant that the data have not yet been fully refined. Sufficient supplementary data must be provided for the referee to judge whether the 'not-fully-refined' structure does indeed prove the desired point, and care should be taken not to overstate the case—for example, by reporting bond lengths to very high degrees of apparent precision when the *R*-factors are poor. Authors must indicate in the paper or the supplementary data the justification for publishing without full refinement; they should complete the refinement and publish the work in full later. In the communication only brief details of the structure, appropriate to the quality of the data, will be expected, but coordinates *etc.* will be deposited with CCDC (or Bonn).

(e) In many cases the structure referred to in a communication will be fully refined. The communication can then be considered to fulfil the archival function, and the structure determination may not require further detailed refereeing when presented as part of a full paper. In the full paper, the author's purpose will then be served by a simple reference back to the original communication. However, if the crystallography is discussed again at any length in the full paper, the data should be re-presented to the referees in full, and re-published if considered necessary.

(f) Even for crystal structure determinations that authors wish to regard as 'unpublished' as far as the communication is concerned, and which are peripheral to the main theme (*e.g.* confirming the structure of an intermediate in an organic synthesis when the structure of the final product has been unambiguously determined by other means), authors are encouraged to submit the supplementary material mentioned in section (c).

(g) For more detailed information, see Instructions for Authors in Issue No. 1 of *J. Chem. Soc., Dalton* or *Perkin Trans.* each year.

(h) To assist the Cambridge Crystallographic Data Centre, authors are requested to complete as much of the Abstract Form given on p. 5 as is possible for each structure determination. This form may be photocopied; alternatively copies are available from the editorial staff.

(i) As an alternative to the printed material, authors are encouraged to supply data for the Cambridge Crystallographic Data Centre on diskette or by electronic mail. Data on *diskette* should be sent to the RSC editorial office when the manuscript is accepted for publication; files should be standard ASCII and full details of disk and file type (*e.g.* CIF, SHELX) should be supplied. Authors wishing to send data by *electronic mail* should inform the editorial office of their intention when the manuscript is accepted. They will be told when the paper is published, and should send the data (to JANET address DGW1@UK.AC.CAM.PHX) at that stage.

CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM

Compound Name
Diagram *(conventional chemical structural diagram)*
Formula *(each residue to be formulated ,eg.* $C_2H_3O_2^-$, Na^+, $2H_2O$*)*

a(Å) *with estimated error*		*b*(Å) *with estimated error*		*c*(Å) *with estimated error*	
alpha(deg.)*with estimated error*		beta(deg.) *with estimated error*		gamma(deg.) *with estimated error*	
Space Group	Z	R-factor(s) R wR	Temp(K)	Radiation ☐ X ☐ N	Powder Data Yes ☐ No ☐
Intensity Measurement ☐ densit. ☐ diffr. ☐ other(*specify*)			Volume(Å^3)	Mol. Weight	Mp(°C)
Absolute Configuration Determined ☐ Yes ☐ No		Colour CAS RN		Dm (g cm^{-3}) Dx (g cm^{-3})	
Polymorph Indicator *(eg. low-temp. form)*					
Drug *(indicate, where appropriate, type of drug, activity, etc.)*					
Disorder *(specify nature of disorder with reference to atom labels in coordinate list)*					