JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANSACTIONS

Instructions for Authors (1996)

CONTENTS

1.0 General Policy

The *Journal of the Chemical Society* is a medium for reporting selected original and significant contributions to new chemical knowledge. Articles which do not present original work (*e.g.* reviews) will not normally be considered for publication in the *Journal*.

All contributions are judged on the criteria of (*i*) originality and quality of scientific content and (*ii*) appropriateness of the length to content of new science. Thus, papers reporting results which would be routinely predicted or result from application of standard procedures or techniques are unlikely to prove acceptable in the absence of other attributes which themselves make publication desirable.

Although short articles are acceptable, the Society strongly discourages fragmentation of a substantial body of work into a number of short publications. Unnecessary fragmentation will be a valid reason for rejection of manuscripts.

1.1 Conditions Governing Acceptance

Contributions which have appeared or have been accepted for publication with essentially the same content in another journal or which incorporate freely available printed work will not be published in the *Journal* except by permission of the Council. This restriction does not apply to results previously published in materially abbreviated form, as a paper presented at a symposium, as a preliminary communication (*e.g.* to *Chemical Communications*), as a letter to the Editor of some other periodical, or as a patent. However, the acceptance of a contribution to *Chemical Communications* (or a communication in the *Transactions*) does not guarantee that the corresponding full paper will be accepted for the *Journal*; although publication of a full account is strongly encouraged, its acceptability will depend on whether or not it contains significant new details, new interpretations, or new results.

Contributions are considered from members and non-members of the Society.

Contributions are accepted by the Society on the understanding that the authors (*a*) have obtained any necessary authority for publication, and (*b*) will execute a formal licence granting the Society exclusive licence under any copyright therein.

Authors are solely responsible for the factual accuracy of their contributions.

Since the Society reserves the right to retain all typescripts sent to it, authors are advised to keep copies. When contributions have been submitted for publication the authors are not at liberty, save by permission of the Society, to withdraw or delay them or to publish them elsewhere until after publication by the Society.

1.2 Submission of Manuscripts

Typescripts should be addressed to: The Managing Editor, *Perkin Transactions 1* or *2*, The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge UK CB4 4WF. North American authors should submit *Perkin Communications* and *Articles* to: Professor Tomas Hudlicky, *North American Associate Editor*, Department of Chemistry, University of Florida, PO Box 117200, Gainesville, FL 32611-7200, USA.

Authors are requested to indicate, at the time of submission, the Journal for which the manuscript is intended.

Four copies of the typescript (a top copy and three good quality copies) are required. (Manuscript pages should be numbered.) Copies of any related, relevant, unpublished material should also be provided.

All authors submitting work for publication are required to sign an exclusive copyright licence. All submissions should be accompanied by a completed form (a blank for photocopying is reproduced at the end of these instructions), without which publication cannot proceed.

Rapid publication is aided by careful preparation of text and illustrations and strict adherence to the format and conventions of individual *Transactions* as laid down in these Instructions for Authors.

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.

Owing to the non-availability of many referees in July–August each year, authors are advised to limit their submissions during this period to minimize delays.

2.0 Administration and Publication Procedure

Receipt of a contribution for consideration will be acknowledged immediately by the Editorial Secretary. The acknowledgement will indicate the paper reference number assigned to the contribution. Authors are particularly asked to quote this number on all subsequent correspondence.

The paper is sent simultaneously to at least two referees, whose names are not disclosed to the authors. On the basis of the referees' reports, the Editor decides whether the paper is suitable for publication, either unchanged or after appropriate revision [new receipt dates are issued to revised versions that take longer than three weeks (six weeks from outside Europe) to reach us]. This decision and relevant comments of the referees are communicated to the author. Differences of opinion are mediated by the Editor, possibly after further consultation with referees.

When rejection of a paper is recommended, the Editor informs the author and returns the top copy of the manuscript. Authors have the right to appeal to the Editorial Board if they regard a decision to reject as unfair.

Acceptance of a paper is confirmed prior to the edited manuscript being sent to the typesetter. The author receives two copies of proofs, together with the edited manuscript and reprint order form. The Society supplies 50 reprints free of charge.

One corrected proof *and* the manuscript should be sent to the Editor. Checking of proofs is the author's responsibility (although the Editor will carry out a further check before publication) and particular attention should be paid to numerical data, both in tables and in the text, references, structural formulae and diagrams.

An author may be required to pay the cost of any extensive changes made by him or her at proof stage (other than the correction of printer's errors). So far as possible, essential changes should be made without altering the length of the text, or at the end of a paragraph. The standard signs for proof correction set out in British Standard BS 5261: Part 2 (1976) may be used: these are conveniently summarized in the pamphlet 'Authors' Alterations Cost Money and Cause Delay . . .' which can be purchased from the British Printing Industries Federation, 11 Bedford Row, London, WC1R 4DX UK. However, the author may prefer simply to put a line through the incorrect characters and write the correct version in the margin. Corrections should be made in ink, clearly and without ambiguity and any queries from the printer or editorial staff on the manuscript or proof should be answered fully.

3.0 Perkin Communications

Preliminary accounts of novel and significant work of exceptional interest may be published in *Perkin Transactions 1* and *2* in Communication form. Work in any branch of organic chemistry may be considered. Material of wide general appeal is more appropriately submitted to *Chemical Communications*; *Perkin Communications* is intended for work of a more specialist nature. **Brief details of key experiments, *e.g.* for a new synthetic procedure, must be included**, but extensive spectroscopic and other supporting experimental data are not required; such data may be provided as supplementary information for the referees. Descriptions and data for routine procedures should *not* be included. Otherwise the criteria governing acceptance are essentially the same as for *Chemical Communications*. Full papers based upon Communications will be acceptable subsequently provided that they represent a substantial amplification and extension of the original material.

Individual articles must be as brief as possible [normally less than two printed pages (1200 words or the equivalent)]. **The summary must be restricted to one sentence only**. The format and style of presentation should be the same as for a full paper.

When submitting a manuscript intended for consideration as a communication, **authors should include a brief statement justifying the need for rapid publication of the work**.

In order to achieve rapid publication, failure of an author to produce a revised script in response to referees' comments within two weeks will be regarded as a withdrawal of the Communication. Furthermore, proof corrections received more than two weeks after despatch of proofs by the printer will not be incorporated.

4.0 Presentation of Papers

Every latitude, consistent with brevity, in the form and style of papers is permitted and no rigid pattern for either is prescribed. Nevertheless, adherence to the methods outlined in this section is recommended unless there is good reason for deviation.

4.1 Organization of Material

4.1.1 *Title*.—The choice of a title for a paper is of the greatest importance, since it is from the title that the important key-words used in information retrieval are taken. Not only should the title clearly and accurately indicate the content of that paper but also it should be as specific as the content and emphasis of the work permit. Brevity in a title, though desirable, should be balanced against its accuracy and usefulness.

The use of abbreviations, symbols and formulae in a title is discouraged; such terms should be written out in full unless they are extremely cumbersome.

The preceding part of a series must be referred to (as reference 1) in the title, in the form:

> Pyrazine chemistry. Part 13.[1] Preparation and reactions of pyrazine *N*-oxides.

The corresponding reference should be in the form:

> 1 Part 12, P. G. Sammes and A. C. Weedon, *J. Chem. Soc., Perkin Trans. 1*, 1979, 3053.

When the preceding part has been submitted to the Society but is not yet published, the paper reference number should be given.

4.1.2 *Summary*.—Every paper for the Journal 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 a reader a clear idea of what has been achieved. The summary should be essentially independent of the main text; however, names or partial names of compounds may be accompanied by the numbers referring to the corresponding displayed formulae in the body of the text.

Examples:

> Apetalactone, a new triterpene lactone isolated from *Calophyllum apetalum* Willd, has been shown to be 28-hydroxy-3,4-secofriedelano-3,4-lactone **2a**.
>
> The synthesis of (*Z*)- and (*E*)-1-azido-1,4-diphenylbut-1-ene **6a** and **b** is described and the products of their

thermal decomposition are reported. The synthesis of 5*H*-pyrrolo[1,2-*a*]azepine **2** and of 7*H*-pyrrolo[1,2-*a*]azepin-7-one **3** *via* the common dihydroazepinone intermediate **11** is also described.

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

4.1.4 *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.

4.1.5 *Experimental Section.*—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.

4.1.6 *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, Dr, Professor, *etc.*, should be given but not degrees.

4.1.7 *Bibliographic References.*—These should be given on a separate sheet at the end of the manuscript; for details see section 4.7.

4.1.8 *Graphical Abstract.*—A representative scheme or structural formulae should be given for the contents list. No more than one sentence of text may be used. The maximum space available is 4 × 9.5 cm. Authors are advised to consult a recent copy of the Journal for examples.

4.2 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.

(*a*) Unnecessary division of work into separate parts of a series of papers.

(*b*) Submission of fragmentary work which can be included in a larger article.

(*c*) Undue elaboration of hypotheses.

(*d*) Over-detailed and verbose exposition of ideas.

(*e*) 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.

(*f*) Duplication of data in text, tables and figures, *etc.*

(*g*) Inclusion of details of the preparation of simple derivatives such as esters, semicarbazones, *etc.*, and slight variations of essentially the same technique. (Unless critical, quantities are superfluous in such cases; only an indication of reagents and perhaps the conditions used is required.)

4.3 Linguistic and Typographical Conventions

4.3.1 *Grammar and Spelling.*—Standard English spelling is used (Oxford English Dictionary). Latitude with respect to alternative spellings is allowed, but consistency should be maintained within a paper. Difficult grammatical points may be elucidated by reference to Fowler's Modern English Usage.

4.3.2 *Abbreviations.*—The following common initial letter abbreviations may be used without definition: bp, mp, CD, EPR, GLC, IR, NMR, ORD, TLC, UV, v/v, w/w. Other such abbreviations should be defined at first mention, as should abbreviations for reagents, *etc.*

4.3.3 *Punctuation.*—Punctuation follows standard English practice; the following conventions are observed.

(*a*) The 'nesting' order for parentheses, square brackets, and braces is {[()]}.

(*b*) Punctuation follows, rather than precedes parentheses, *e.g.* 'mp 234 °C (decomp.),' and not 'mp 234 °C, (decomp.)'.

(*c*) A colon is used to separate a ratio as in 1:20—not a solidus 1/20.

(*d*) Parenthetical expressions of the same physical quantity in different units are separated by a comma, *e.g.* (3.9 g, 0.1 mol), (30 cm^3, 1 mol); expressions of different physical quantities are separated by a semicolon, *e.g.* (2.9 g cm^{-3}; 30 cm^3).

4.3.4 *Use of Italics.*—(*a*) Foreign words and phrases and Latin abbreviations are given in italics: *e.g., in toto, in vivo, ca., cf., i.e., etc.*

(*b*) 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: fullstops are not to be associated with letter prefixes.)

Examples:

> *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*-cyclohexane-1,2-diol, *gem*- and *vic*-diols, benzil (*E*)-oxime, 3-*O*-methyl-L-*glycero*-tetrulose.

At the beginning of a sentence the first roman letter after the prefix is capitalized: 'D-*glycero*-D-*gluco*-Heptose was subjected . . .' and 'β-*p*-Tolylchalcone gave . . .'

(*c*) The scientific names of genera and species are italicized.

(*d*) The names of periodicals or their abbreviations are set in italics.

4.3.5 *Headings.*—(*a*) Main sections (Introduction, Experimental, Discussion, *etc.*): centre-heading, bold, initial capital letter for first word only, no final full stop.

(*b*) Main side-heading: bold, initial capital for first word only, no final full stop.

(*c*) Subsidiary side-heading: indented, bold, initial capital letter for first word only, final full stop, text run on from heading.

(*d*) Further subdivision: indented, italic, initial capital for first word only, final full stop and dash, text run on from heading.

Examples:

Experimental

Preparation of aliphatic oximes

Oxime O-alkyl derivatives. (*a*) Acetaldehyde oxime (100 g) was dissolved . . .

Density of the alcohol at 295 K
The series of aliphatic alcohols . . .

4.4 Formulae and Figures

The purpose of all illustrative matter in a paper is to clarify the arguments and descriptions rather than to duplicate them. The Society 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.

All formulae and figures should be clearly drawn, and in the case of figures, provided with captions; the latter should be typed on a separate sheet. Since all formulae carry key numbers by which they are identified, unless they form part of the running text or unless they are part of a scheme which itself has a caption, they are not generally further described. Blocks of formulae do not need captions.

4.4.1 *Structural Formulae.*—(*a*) Only those formulae which are displayed should be given key numbers. In other cases compounds should be referred to by name.

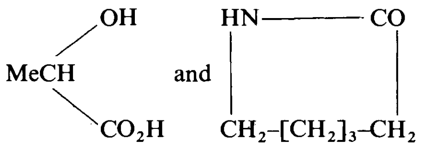
(*b*) Formulae should be numbered with bold arabic numerals, **1**, **2** and **3** *etc.*, in the order in which they are displayed and not in the order of mention in text.

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

(*d*) Structural or displayed formulae must be carefully and accurately drawn or typed on a separate sheet, rather than inserted into the text, although a marginal indication of where they are to go in the text is desirable.

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

$\mathrm{HO{-}CHMe{-}CO_2H}$ and $\overline{\mathrm{NH{-}[CH_2]_5{-}CO}}$ rather than



$$\mathrm{MeCH}\left\langle\begin{array}{l}\mathrm{OH}\\ \mathrm{CO_2H}\end{array}\right. \quad \text{and} \quad \begin{array}{l}\mathrm{HN}\text{————}\mathrm{CO}\\ \mathrm{CH_2{-}[CH_2]_3{-}CH_2}\end{array}$$

(*f*) Hyphens may be used to indicate bonds between the atoms of the backbone chain of a compound. The symbol of each element of that chain is preceded by a hyphen and followed by the symbols or formulae of the atoms or groups that are attached to it (parentheses being used where necessary to enclose compound groups), *e.g.* $o\text{-}\mathrm{HO{-}C_6H_4{-}CH_2{-}NH_2}$ and $\mathrm{CH_2Cl{-}CH(OH){-}CO_2H}$.

Hyphens are unnecessary with groups that are indicated by an abbreviation (*e.g.* Me, Et, *etc.*). They may be omitted in other cases also, where no ambiguity results.

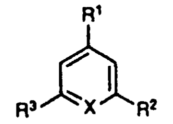
Repeating sequences of a backbone composite group are enclosed in square brackets and their number is indicated by an inferior multiplier, *e.g.* $\mathrm{HO[CH_2]_4NH_2}$, but $\mathrm{HO[CH_2]_4N(CH_2OH)_2}$.

(*g*) Steric conventions must be observed, notably for steroids, triterpenes and carbohydrates. The Society uses wedges (◀) or heavy lines (—) rather than blocked circles (●), and broken lines in the form - - - -.

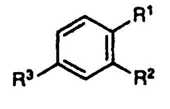
(*h*) The abbreviations Me, Et, Pr, $\mathrm{Pr^i}$, Bu, $\mathrm{Bu^i}$, $\mathrm{Bu^s}$, $\mathrm{Bu^t}$, Ph, Ac, Alk, Ar and Hal, should be used except when the group is involved in the reaction described. Other special symbols, if used, require an explanatory footnote.

(*i*) One variable univalent substituent is indicated by R; when more than one independently variable general substituent is present, R^1, R^2 and R^3 should be used (not R, R^1, R^2, R^3; or R_1, R_2 and R_3 which indicate 1 × R, 2 × R, *etc.*).

(*j*) Often it is desirable to use one formula to represent a number of related compounds (or classes of compounds) by the use of one or more independently variable substituents. It is preferable to give each compound thus represented a separate key number rather than subdivide individual key numbers by alphabetical suffixes *i.e.* **1a**, **1b**, **1c** *etc.*



1 $R^1 = R^2 = \mathrm{Ph}$, $R^3 = \mathrm{Me}$, $X = O^+$
2 $R^1 = \mathrm{Me}$, $R^2 = R^3 = \mathrm{Ph}$, $X = S^+$



3 $R^1 = \mathrm{Me}$, $R^2 = \mathrm{Ph}$, $R^3 = \mathrm{PhCO}$
4 $R^1R^2 = \mathrm{CO{-}O{-}CO}$, $R^3 = \mathrm{Ph}$

The use of more than four independently variable substituents or atoms on one generalized formula is discouraged.

(*k*) Once a formula has been displayed it is permissible to employ its key number in later reaction schemes or equations rather than to re-display the formula.

(*l*) Displayed formulae, unless they are capable of being typed on one line [see point (*e*) above], should not be included in tables; they should be displayed elsewhere and their numbers should be used in the table itself.

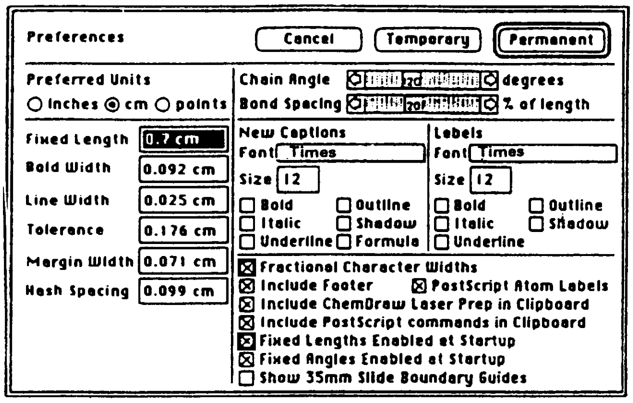
(*m*) The key number for a compound may be used in the cursive text to avoid repetition of long chemical names; this device must not be used to excess. In general it is preferred if the key number is qualified by a partial name as in the following example:

'Pyolin **1** was oxidized by permanganate to the oxo acid **2**, the methyl ester **3** of which with methylmagnesium iodide gave the normal product **4**.'

(*n*) 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.

4.4.2 *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 in the journals as submitted, but it is expected that this route will minimize 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 preference settings to be used are as follows: fixed length 0.7 cm; line width 0.025 cm; bold width 0.092 cm; hash spacing 0.099 cm; bond spacing 20% of length; font Times 12 pt; single width bold and **dashed lines** should be used to show stereochemistry. The page set-up for preparation of drawings



Preferences

Cancel | Temporary | Permanent

Preferred Units
○ inches ● cm ○ points

Chain Angle 120 degrees
Bond Spacing 20 % of length

Fixed Length 0.7 cm
Bold Width 0.092 cm
Line Width 0.025 cm
Tolerance 0.176 cm
Margin Width 0.071 cm
Hash Spacing 0.099 cm

New Captions
Font Times
Size 12
☐ Bold ☐ Outline
☐ Italic ☐ Shadow
☐ Underline ☐ Formula

Labels
Font Times
Size 12
☐ Bold ☐ Outline
☐ Italic ☐ Shadow
☐ Underline

☒ Fractional Character Widths
☒ Include Footer ☒ PostScript Atom Labels
☒ Include ChemDraw Laser Prep in Clipboard
☒ Include PostScript commands in Clipboard
☒ Fixed Lengths Enabled at Startup
☒ Fixed Angles Enabled at Startup
☐ Show 35mm Slide Boundary Guides

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.

4.4.3 *Figures.*—(*a*) Figures must bear on the back the names of the authors, the title of the paper (abbreviated if necessary), and the number of the figure.

(*b*) Figures must be in black ink, on board, white smooth cartridge paper, tracing linen, plastic film (it is essential that the special plastic ink developed for this is used), or graph paper with faint blue lines (red or brown lines must not be present as these may be reproduced by the photographic process employed). Since lines must be black and sharp, photostats or similar prints are often not suitable. If paper is used, it must be strong enough to withstand repeated handling.

(*c*) Lettering and numerals must be in blue pencil (not red or black pencil or ink) clearly legible but not so heavily scored as to make a permanent impression on the paper or board.

(*d*) When the figures are large (more than 20 × 25 cm), smaller copies (which may be rough, as long as they are clear) should be supplied for submission to the referees; editing will not be undertaken, however, before the final figures are received.

(*e*) Figures should be drawn about three times the required size, with lines thick enough to withstand photoreduction. Particular care should be taken with pairs of crystal structure diagrams for stereoscopic viewing: for good reproduction an adequate line thickness is essential.

(*f*) The expression used to define the numerical values of a physical quantity plotted on a graph should be dimensionless, *e.g.* $\ln(p/\mathrm{atm})$, $10^3(T/\mathrm{K})^{-1}$.

(*g*) Figures are numbered consecutively Fig. 1, Fig. 2, *etc.* (in arabic numerals).

(*h*) Since figures represent an uneconomical use of space their number and size should be kept to a minimum. Figures and tables for the same values are discouraged.

4.5 Presentation of Experimental Data

4.5.1 *Tables.*—If there is extensive reference to any particular data in the text, presentation of the data in tabular form is preferred. It is difficult to give general rules for the economical layout of tables, but authors will find it helpful to consult recent issues of the *Journal* for examples. A layout taking up the full width of the printed page, with repetition of column headings if necessary, is normally preferred to a lengthy half-page-width presentation. Columns containing very few entries are wasteful of space and better replaced by footnotes.

When tables (and figures) are reproduced in the Journal, they will be positioned at the top or the bottom of a printed page, as near as possible to their first mention.

Column headings should be brief, as their width, rather than that of the entries beneath them, often determines the number of columns that can be accommodated.

Column headings should be in accord with the conventions associated with SI; thus the expression at the head of a column of numerical values of a physical quantity should be dimensionless, *i.e.* the quotient of the symbol for the physical quantity and the symbol for the unit used, *e.g.* p/atm, or the symbol for a dimensionless physical quantity, *e.g.* pV^{G}, or some mathematical function of such a number, *e.g.* $\ln(p^{\mathrm{m}}/\mathrm{atm})$.

Example:

$\theta/°\mathrm{C}$	T/K	$10^3\mathrm{K}/T$	p/atm	$\ln(p/\mathrm{atm})$
−51.60	216.55	4.6179	5.112	1.6316
	$V_{\mathrm{m}}^{\mathrm{G}}/\mathrm{cm^3\ mol^{-1}}$		$pV_{\mathrm{m}}^{\mathrm{G}}/RT$	
	3 177.6		0.9142	

Space requirements may favour the use of a horizontal rule, *e.g.* $\dfrac{V_{\mathrm{m}}^{\mathrm{G}}}{\mathrm{cm^3\ mol^{-1}}}$ rather than an oblique stroke.

Tables should be arranged such that values are read down the columns and not across the page.

4.5.2 *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.* '$[\alpha]_{\mathrm{D}}$ values are given in 10^{-1} deg cm^2 g^{-1}'. Shown in the form $[\alpha]_{\mathrm{D}}^{22}$ −22.5 (*c* 0.95 in EtOH), *i.e.* concentration and solvent in parentheses.

Refractive index. Given in the form n_{D}^{22} 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 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 $\lambda_{\max}$(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: $\lambda_{\max}$(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: $\nu_{\max}$/cm^{-1} 3460 and 3330 (NH), 2200 (conj. CN), 1650 (CO) and 1620 (C=N). 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; underlining for italics can be used to specify the nuclei concerned (*e.g.* $CH_3C\mathit{H}_2$). 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.

Mass spectrum. 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 $\longrightarrow$ 174), 147 (176 $\longrightarrow$ 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. Authors should note in particular the specification of quantities in parentheses after the names of reagents and the use of the past tense.

Oxidation of the lactone 16

A solution of the lactone **16** (40 mg, 16 mmol) in acetone (5 cm^3) was oxidized with Jones' reagent (16 mmol) at room temperature for 4 h. The solution was poured into cold water and extracted with chloroform. The extract was washed with aqueous sodium hydrogen carbonate and water, dried, and evaporated to dryness. Chromatography on silica gel with ethyl acetate–light petroleum (bp 40–60 °C) (1 : 1) as the eluent yielded *vulgarin* **21** (11 mg, 27%), mp 176–177 °C (Found: C, 68.35; H, 7.75. $C_{15}H_{20}O_4$ requires C, 68.15; H, 7.5%); $[\alpha]_D^{22}$ +39 (*c* 0.3 in $CHCl_3$); $\nu_{max}(CHCl_3)/cm^{-1}$ 3520 (OH), 1780 (γ-lactone) and 1675 (α,β-unsaturated ketone); λ_{max}(EtOH)/nm 215; δ_H(90 MHz; $CDCl_3$) 1.23 (3 H, s, 10-Me), 1.28 (3 H, d, *J* 7, 11-Me), 1.55 (3 H, s, 4-Me), 2.36 (1 H, d, *J* 10, 5-H), 4.25 (1 H, dd, *J* 9 and 10, 6-H), 5.90 (1 H, d, *J* 10, 2-H) and 6.62 (1 H, d, *J* 10, 3-H); *m*/*z* 264 (M^+, 100%) and 246 (M^+ − 18).

If desired, an alternative, tabular presentation of selected data may be used; an example is shown (Table 0).

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

4.6 Authentication 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. 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 are not available, appropriate evidence which is convincing to an expert in the field may be acceptable, but authors should include, for the referees, a brief explanation of the special nature of their problem.

Spectroscopic information necessary to the assignment of structure should normally 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 a Supplementary Publication where their importance does not justify their inclusion in the published paper.

4.7 Bibliographic References and Footnotes

A clear distinction is made between bibliographic references and footnotes. The latter are 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. Such footnotes are referred to with the following symbols: *, †, ‡, §, ¶, ||, *etc.* [*Note:* since an asterisk is used to indicate the author to whom correspondence should be addressed, its use early on in a paper is not advised; a dagger (†) is preferred.]

Bibliographic reference to the source of statements in the text is made by use of *superior numerals* at the appropriate place. The references themselves are given at the end of the final printed

Table 0 Analytical data for the thioamides **28**–**30**

Compound (Formula)	Yield (%)	Solvent	Mp/°C (decomp.)	Found (%) (Required) C	H	N
28	69	MeOH	168–169	44.1	2.75	2.3
($C_{22}H_{16}INO_5S_3$)				(44.2	2.7	2.3)
29	65	MeOH	168–170	52.4	3.0	2.7
($C_{22}H_{16}ClNO_5S_3$)				(52.2	3.2	2.8)
30	63	aq. Me_2CO	162–163	45.35	2.9	2.3
($C_{23}H_{18}INO_2S_3$)				(45.2	2.0	2.3)

text. It is essential that they are numbered in the order in which they are cited in the text.

The position of the superior numeral should be chosen with care, particularly when it does not follow an author's name. If placed adjacent to punctuation, the numeral should normally be placed after the punctuation mark, *e.g.* 'This compound was shown to be the dienone,^{3} which . . .'.

Particular care is necessary where a reference number is likely to be confused with a superscript numeral indicating a power index: '. . . which gave a value of 2.3 cm^3 . . . should be written as '. . . which gave a value^3 of 2.3 cm' or '. . . which gave a value of 2.3 cm (ref. 3)'.

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 recognized systems. The list of CASSI-style abbreviations covers many of the journals received in the library of the Royal Society of Chemistry. 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**.

Books. Titles of books are cited in italics and the author(s), title, publisher, town, date (or edition, if more than one has been published) and page number (if required) must be given in that order:

I. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, Wiley, Chichester, 1978, p. 55.

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.

Patents. Patents should be indicated in the forms: BP 367 450, 367 455–7, USP 1 171 230. GP 436 112–4, Jap P 20 101. Dates are indicated thus: BP 666 776/1956. Patents which are applied for must always be given a year, *e.g.* BP Appl. 102/1982. Chemical Abstracts references should be given, *e.g.*, BP 2018 253/1978 (*Chem. Abstr.*, 1980, **93**, 45990).

Reports and Bulletins, etc.

G. M. Sheldrick, SHELX-76, Program for Crystal Structure Determinations, University of Cambridge, 1976.

J. B. Pedley and J. Rylance, Sussex-NPL Computer Analysed Thermochemical Data: Organic and Organometallic Compounds, University of Sussex, 1977.

Material presented at meetings.

S. Clementi, presented at the Second European Symposium on Organic Chemistry (ESOC II), Stresa, 1981.

M. Prevost and R. Bugarel, *Proceedings of the International Seminar on Thermochemical Energy Storage*, Stockholm, 1980, p. 95.

Theses.

A. D. Mount, Ph.D. Thesis, University of London, 1982.

Reference to unpublished material. For material presented at a meeting, congress, or before a Society, *etc.*, but not published, the following form is used:

1 A. R. Jones, presented in part at the 28th Congress of the International Union of Pure and Applied Chemistry, Vancouver, August, 1981.

For material accepted for publication, but not yet published, the following form is used:

2 A. R. Jones, *J. Chem. Soc., Perkin Trans. 1*, in the press.

If the paper has been submitted to the Society, the paper number should be given:

3 A. R. Jones, *J. Chem. Soc., Perkin Trans. 1*, in the press (4/00556A).

For material submitted for publication but not yet accepted the following form is used:

4 A. R. Jones, submitted for publication in *Angew. Chem.*

For personal communications the following is used:

5 G. B. Ball, personal communication. (*Note:* the form G. B. Ball, private communication, is inappropriate.)

If material is to be published but has yet to be submitted the following form is used:

6 G. B. Ball, unpublished work.

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

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.

For Chinese and Spanish authors all names should be given as in the original, since the patronymic is not always given last in these languages. If co-authors are to be collectively cited, as in 'Smith and co-workers' or 'Smith *et al.*,' the latter form is inappropriate unless the individual name 'Smith' appears first among the authors named in the original.

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

1 A. B. Jones, *J. Chem. Soc., Perkin Trans. 2*, 1975, 234.

2 A. B. Jones, *J. Chem. Soc., Perkin Trans. 2*, 1977, 123; 1978, 234.

3 A. B. Jones, *J. Chem. Soc., Perkin Trans. 1*, 1977, 123; *J. Am. Chem. Soc.*, 1956, **78**, 1234.

4 A. B. Jones, *J. Chem. Soc.*, 1956, 234; A. B. Jones and C. D. Brown, *J. Chem. Soc. B*, 1967, 234, 1077; 1968, 599.

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

If only one paper from a composite reference is required for citation later, then two numbers may be assigned to the first citation (*e.g.* Jones^{1,2}); alternatively, long composite references may be divided by letters, *e.g.*:

(*a*) A. B. Jones, *J. Chem. Soc., Perkin Trans. 1*, 1978, 467; (*b*) A. B. Jones and C. D. Brown, *J. Chem. Soc., Perkin Trans. 2*, 1979, 234.

A. B. Jones, *J. Chem. Soc. C*, (*a*) 1967, 267; (*b*) 1968, 1742; (*c*) *etc.*

A composite reference may cite a previous reference in the form:

12 A. B. Jones, *J. Chem. Soc.*, 1956, 234; C. D. Brown, ref. 5.

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

4.8 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.

In order to encourage authors to use IUPAC nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given:

Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H, Pergamon, Oxford, 1979 edn.

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

Journal Abbreviations

Acc. Chem. Res.
Acta Biochim. Biophys. Acad. Sci. Hung.
Acta Biochim. Pol.
Acta Chem. Scand., Ser. A
Acta Chem. Scand., Ser. B
Acta Chim. Acad. Sci. Hung.
Acta Crystallogr.. Sect. A
Acta Crystallogr., Sect. B
Acta Crystallogr., Sect. C
Acta Phys. Chem.
Acta Vitaminol. Enzymol.
Adv. Alicyclic Chem.
Adv. Carbohydr. Chem. Biochem.
Adv. Catal.
Adv. Chem. Phys.
Adv. Colloid Interface Sci.
Adv. Enzymol. Relat. Areas Mol. Biol.
Adv. Fluorine Chem.
Adv. Free-Radical Chem.
Adv. Heterocycl. Chem.
Adv. Inorg. Bioinorg. Mech.
Adv. Inorg. Chem. Radiochem.
Adv. Lipid Res.
Adv. Macromol. Chem.
Adv. Magn. Reson.
Advan. Mater.
Adv. Organomet. Chem.
Adv. Org. Chem.
Adv. Photochem.
Adv. Phys. Org. Chem.
Adv. Protein Chem.
Adv. Quantum Chem.
Adv. Struct. Res. Diffr. Methods
Afinidad
Agric. Biol. Chem.
AIChE J.
Ambix
Am. J. Pharm.
Am. J. Sci.
An. Acad. Bras. Cienc.
Anal. Biochem.
Anal. Chem.
Anal. Chim. Acta
Anal. Lett.
Analyst (London)
Angew. Chem.
Angew. Chem., Int. Ed. Engl.
Angew. Makromol. Chem.
Ann. Acad. Sci. Fenn., Ser. A2
Ann. Chim. (Paris)
Ann. Chim. (Rome)
Ann. Endocrinol.
Ann. N.Y. Acad. Sci.
Ann. Pharm. Fr.
Ann. Soc. Sci. Bruxelles, Ser. 2
Annu. Rep. Anal. At. Spectrosc.
Annu. Rep. Med. Chem.
Annu. Rep. N.M.R. Spectrosc.
Annu. Rep. Prog. Chem., Sect. A, Inorg. Chem.
Annu. Rep. Prog. Chem., Sect. B, Org. Chem.
Annu. Rep. Prog. Chem., Sect. C, Phys. Chem.
Annu. Rev. Biochem.
Annu. Rev. Ind. Eng. Chem.
Annu. Rev. Phys. Chem.
Appl. Spectrosc.
Arch. Pharm. Chemi, Sci. Ed.
Arch. Pharm. (Weinheim, Ger.)
Arm. Khim. Zh.
Arzneim.-Forsch.
Aspects Homogeneous Catal.
Aust. J. Biol. Sci.
Aust. J. Chem.

Ber. Bunsenges. Phys. Chem.
Biochem. Biophys. Res. Commun.
Biochem. Educ.
Biochemistry
Biochemistry (Eng. Transl.)
Biochem. J.
Biochem. Pharmacol.
Biochem. Prep.
Biochem. Soc. Trans.
Biochim. Biophys. Acta
Biochimie
Biofizika
Bioinorg. Chem.
Biokhimiya
Bioorg. Chem.
Bioorg. Khim.
Biopolymers
Biotechnol. Bioeng.
Boll. Soc. Ital. Biol. Sper.
Br. J. Pharmacol.
Br. Polym. J.
Bull. Acad. Sci. USSR, Div. Chem. Sci.
Bull. Chem. Soc. Jpn.
Bull. Inst. Chem. Res., Kyoto Univ.
Bull. Pol. Acad. Sci., Chem.
Bull. Soc. Chim. Belg.
Bull. Soc. Chim. Fr.
Bunseki Kagaku

Can. J. Biochem.
Can. J. Chem.
Can. J. Chem. Eng.
Can. J. Pharm. Sci.
Can. J. Phys.
Can. J. Spectrosc.
Carbohydr. Res.
Carbon
Catal. Rev.
Cellul. Chem. Technol.
Cesk. Farm.
Chem. Age (London)
Chem. Ber.
Chem. Br.
Chem. Eng. News
Chem. Eng. Progr.
Chem. Eng. Sci.
Chem. Erde
Chem. Heterocycl. Compd. (Engl. Transl.)
Chem. Ind. (Duesseldorf)
Chem. Ind. Int. (Engl. Transl.)
Chem. Ind. (London)
Chem.-Ing.-Tech.
Chem. Lett.
Chem. Listy
Chem. Nat. Compd. (Engl. Transl.)
Chem. N.Z.
Chem. Pharm. Bull.
Chem. Phys.
Chem. Phys. Carbon
Chem. Phys. Lett.
Chem. Phys. Lipids
Chem. Rev.
ChemSA
Chem. Scr.
Chem. Soc. Rev.
Chem. Tech. (Leipzig)
Chem. Technol.
Chem. Week
Chem. Weekbl.
Chem.-Ztg.
Chem. Zvesti
Chim. Actual.
Chimia
Chim. Ind. (Milan)
Chromatographia
Clin. Biochem.
Clin. Chem. (Winston-Salem, N.C.)
Clin. Chim. Acta
Collect. Czech. Chem. Commun.
Colloid J. USSR (Engl. Transl.)
Colloid Polym. Sci.
Commun. R. Soc. Edinburgh, Phys. Sci.
Comput. Chem.
Coord. Chem. Rev.
CRC Crit. Rev. Biochem.
C.R. Seances Acad. Sci.
Crit. Rev. Anal. Chem.
C.R. Seances Soc. Biol. Ses Fil.
Curr. Sci.

Dokl. Akad. Nauk Arm. SSR
Dokl. Akad. Nauk SSSR
Dokl. Bolg. Akad. Nauk
Dokl. Chem. (Engl. Transl.)
Dokl. Chem. Technol. (Engl. Transl.)
Dokl. Phys. Chem. (Engl. Transl.)
Dopov. Akad. Nauk Ukr. RSR, Ser. B
Dyn. Mass Spectrom.

Educ. Chem.
Electroanal. Chem.
Electrochim. Acta
Elektrokhimiya
Endeavour
Environ. Sci. Technol.
Essays Biochem.
Eur. J. Biochem.
Eur. Polym. J.
Experientia

Faraday Discuss. Chem. Soc.
Faraday Symp. Chem. Soc.
FEBS Lett.
Finn Chem. Lett.
Fiz.-Khim. Mekh. Mater.
Fiz. Met. Metalloved.
Flavour Ind.
Fluorine Chem. Rev.
Fortschr. Chem. Org. Naturst.
Fortschr. Hochpolym.-Forsch.
Fresenius' Z. Anal. Chem.
Fuel

Gazz. Chim. Ital.
Gen. Cytochem. Methods
Ger. Chem. Eng. (Engl. Transl.)
G. Microbiol.

Helv. Chim. Acta
Heterocycles
High Energy Chem. (Engl. Transl.)
Hua Hsueh
Hua Hsueh Tung Pao
Huaxue Tongbao
Huaxue Xuebao
Hung. J. Ind. Chem.

Ind. Eng. Chem., Fundam.
Indian J. Biochem. Biophys.
Indian J. Chem., Sect. A
Indian J. Chem., Sect. B
Indian J. Pure Appl. Phys.
Ind. Lab. (Engl. Transl.)
Inorg. Chem.
Inorg. Chim. Acta
Inorg. Mater. (Engl. Transl.)
Inorg. Synth.
Int. Chem. Eng.
Int. J. Appl. Radiat. Isot.
Int. J. Chem. Kinet.
Int. J. Mass Spectrum. Ion Processes
Int. J. Pept. Protein Res.
Int. J. Quantum Chem.
Int. J. Quantum Chem., Symp.
Int. J. Sulfur Chem.
Int. J. Vitam. Nutr. Res.
Intra-Sci. Chem. Rep.
Inz. Chem.
Ion Exch. Solvent Extr.
Isr. J. Chem.
Ital. J. Biochem.
Izv. Akad. Nauk Kaz. SSR, Ser. Khim.
Izv. Akad. Nauk SSSR, Neorg. Mater.
Izv. Akad. Nauk SSSR, Ser. Khim.

J. Am. Chem. Soc.
J. Anal. At. Spectrom.
J. Anal. Chem. USSR (Engl. Transl.)
J. Appl. Chem. Biotechnol.
J. Appl. Chem. USSR (Engl. Transl.)
J. Appl. Crystallogr.
J. Appl. Polym. Sci.
J. Assoc. Public Anal.
J. Biochem. (Tokyo)
J. Biol. Chem.
J. Carbohydr. Chem.
J. Catal.
J. Chem. Educ.
J. Chem. Eng. Data
J. Chem. Inf. Comput. Sci.
J. Chem. Phys.
J. Chem. Res. (M)
J. Chem. Res. (S)
J. Chem. Soc., Chem. Commun.
J. Chem. Soc., Dalton Trans.
J. Chem. Soc., Faraday Trans.
J. Chem. Soc., Perkin Trans. 1
J. Chem. Soc., Perkin Trans. 2
J. Chem. Thermodyn.
J. Chim. Phys. Phys.-Chim. Biol.
J. Chin. Chem. Soc. (Taipei)
J. Chromatogr.
J. Chromatogr. Sci.
J. Colloid Interface Sci.
J. Comput. Chem.
J. Coord. Chem.
J. Cryst. Mol. Struct.
J. Electrochem. Soc.
J. Electrochem. Soc. India
J. Fluorine Chem.
J. Food Sci.
J. Gen. Chem. USSR (Engl. Transl.)
J. Hazard. Mater.
J. Heterocycl. Chem.
J. Histochem. Cytochem.
J. Indian Chem. Soc.
J. Indian Inst. Sci.
J. Inorg. Chem. USSR (Engl. Transl.)
J. Inst. Chem. (India)
J. Inst. Fuel
J. Labelled Compd. Radiopharm.
J. Lipid Res.
J. Liq. Chromatogr.
J. Macromol. Sci., Chem.
J. Macromol. Sci., Phys.
J. Magn. Reson.
J. Mater. Chem.
J. Med. Chem.
J. Mol. Biol.
J. Mol. Catal.
J. Mol. Spectrosc.
J. Mol. Struct.
J. Neurochem.
J. Nonmet. Semiconduct.
J. Organomet. Chem.
J. Org. Chem.
J. Org. Chem. USSR (Engl. Transl.)
J. Pharmacol.
J. Pharmacol. Exp. Ther.
J. Pharm. Pharmacol.
J. Pharm. Sci.
J. Photochem.
J. Phys. Chem.
J. Phys. Chem. Ref. Data
J. Phys. Chem. Solids
J. Phys. E.
J. Polym. Sci., Polym. Chem. Ed.
J. Polym. Sci., Polym. Phys. Ed.
J. Polym. Sci., Polym. Symp.
J. Prakt. Chem.
J. Protein Chem.
J. Quant. Spectrosc. Radiat. Transfer
J. Radioanal. Nucl. Chem.
J. Raman Spectrosc.
J. Res. Inst. Catal., Hokkaido Univ.
J. Res. Nat. Bur. Stand., Sect A
J. Sci. Food Agric.
J. Sci. Hiroshima Univ., Ser. A2
J. Sci. Ind. Res.
J. Soc. Leather Technol. Chem.
J. Solid State Chem.
J. Solution Chem.
J. Steroid Biochem.
J. Struct. Chem. (Engl. Transl.)
J. Therm. Anal.

Kagaku Kogaku
Kem.-Kemi
Khim. Geterotsikl. Soedin.
Khim. Ind. (Sofia)
Khim. Prir. Soedin.
Khim. Promst. (Moscow)
Khim. Volokna
Kinet. Catal. (Engl. Transl.)
Kinet. Katal.
Kjemi
Kobunshi Kagaku
Kogyo Kagaku Zasshi
Kolloidn. Zh.
Koord. Khim.
Kristallografiya
Kunstst.-Plast. (Solothurn, Switz.)

Lab. Pract.
Langmuir
Laser Chem.
Liebigs Ann. Chem.
Lipids

Macromolecules
Macromol. Synth.
Magy. Kem. Foly.
Magy. Kem. Lapja
Makromol. Chem.
Meded. Vlaam. Chem. Ver.
Mekh. Polim.
Mem. Fac. Sci. Kyushu Univ., Ser. C
Mem. Inst. Protein Res., Osaka Univ.
Methods Biochem. Anal.
Methods Free-Radical Chem.
Microchem. J.
Mikrochim. Acta
Mol. Cell. Biochem.
Mol. Cryst. Liq. Cryst.
Mol. Phys.
Monatsh. Chem.

Nat. Prod. Rep.
Nature (London)
Naturwissenschaften
Neftekhimiya
New J. Chem.
Nippon Kagaku Kaishi
Nippon Nogei Kagaku Kaishi
Nouv. J. Chim.
Nucleosides, Nucleotides

Oesterr. Chem.-Zig.
Orbital
Organometallics
Org. Magn. Reson.
Org. Mass. Spectrom.
Org. Prep. Proced. Int.
Org. React. (N.Y.)
Org. React. (USSR)
Org. React. Mech.
Org. Synth.

Pak. J. Sci.
Pak. J. Sci. Ind. Res.
Pak J. Sci. Res.
Philos. Mag.
Philos. Trans. R. Soc. London, A
Phosphorus Sulfur
Photochem. Photobiol.
Phys. Chem. Glasses
Phys. Rev.
Phys. Rev. Lett.
Phys. Scr.
Phytochemistry
Pol. J. Chem.
Polyhedron
Polym. Age
Polym. Commun.
Polymer
Polym. Sci. USSR (Engl. Transl.)
Postepy Biochem.
Prikl. Biokhim. Mikrobiol.
Proc. Am. Soc. Brew. Chem.
Process Biochem.
Proc. Indian Acad. Sci., Sect. A
Proc. Indian Acad. Sci., Sect. B
Proc., K. Ned. Akad. Wet., Ser. B
Proc., K. Ned. Akad. Wet., Ser. C
Proc. Natl. Acad. Sci., India, Sect. A
Proc. Natl. Acad. Sci. USA
Proc. R. Soc. Edinburgh, Sect. A
Proc. R. Soc. London, Ser. A
Proc. R. Soc. London, Ser. B
Proc. Soc. Exp. Biol. Med.
Prog. Bioorg. Chem.
Prog. Colloid Polym. Sci.
Prog. Inorg. Chem.
Prog. Med. Chem.
Prog. Nucleic Acid Res. Mol. Biol.
Prog. Nucl. Magn. Reson. Spectrosc.
Prog. Phys. Org. Chem.
Prog. React. Kinet.
Prog. Solid State Chem.
Prog. Stereochem.
Pure Appl. Chem.

Radiat. Phys. Chem.
Radiat. Res.
Radiochim. Acta
Radiokhimiya
React. Kinet. Catal. Lett.
Recent Dev. Chem. Nat. Carbon Compd.
Recent Prog. Horm. Res.
Recherches

Journal Abbreviations (*continued*)

Recl. Trav. Chim. Pays-Bas
Rep. Prog. Appl. Chem.
Rev. Anal. Chem.
Rev. Chim. (Bucharest)
Rev. Phys. Chem. Jpn.
Rev. Port. Quim.
Rev. Roum. Biochim.
Rev. Roum. Chim.
Rev. Sci. Instrum.
Rev. Soc. Quim. Mex.
Russ. Chem. Rev. (Engl. Transl.)
Russ. J. Inorg. Chem. (Engl. Transl.)
Russ. J. Phys. Chem. (Engl. Transl.)

S. Afr. J. Chem.
Science
Sci. Sinica
Sov. Electrochem. (Engl. Transl.)
Sov. J. Bioorg. Chem. (Engl. Transl.)
Spec. Publ. Chem. Soc.
Spectrochim. Acta, Part A
Spectrochim. Acta, Part B
Spectrosc. Lett.
Steroids
Steroids Lipids Res.
Struct. Bonding (Berlin)
Synlett
Synth. Commun.
Synthesis
Synth. React. Inorg. Metal-Org. Chem.

Talanta
Teor. Eksp. Khim.
Tetrahedron
Tetrahedron: Asymmetry
Tetrahedron Lett.
Theor. Exp. Chem. (Engl. Transl.)
Thermochim. Acta
Top. Curr. Chem.
Top. Stereochem.
Trends Biochem. Sci.

Ukr. Biokhim. Zh.
Ukr. Khim. Zh. (Russ. Ed.)
Usp. Khim.
Uzb. Khim. Zh.

Vitam. Horm. (N. Y.)

Xenobiotica

Z. Chem.
Zh. Fiz. Khim.
Zh. Neorg. Khim.
Zh. Obshch. Khim.
Zh. Org. Khim.
Zh. Prikl. Khim. (Leningrad)
Zh. Strukt. Khim.
Z. Naturforsch., Teil A
Z. Naturforsch., Teil B
Z. Naturforsch., Teil C
Z. Phys. Chem. (Munich)
Z. Phys. Chem. (Leipzig)
Z. Vitam., Horm., Fermentforsch.
Z. Wiss. Photogr., Photophys., Photochem.

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

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

Compendium of Chemical Terminology: IUPAC Recommendations, Blackwell, Oxford, 1987.

A listing of all relevant IUPAC nomenclature publications appears as an appendix to these Instructions.

It is recommended that where 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.

4.9 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.).

Guidelines for the publications of the Society. If non-SI units are used for critical data or for quantities measured to a high order of accuracy (as opposed to the rough physical conditions of an experiment), the definitive values will be expressed in SI units as well.

The following will be the guidelines used:

(*a*) A metric system will always be used in preference to a non-metric one.

(*b*) SI will be the standard usage.

(*c*) The units used to record the definitive values of 'critical data' or quantities measured to high degree of accuracy will be SI.

(*d*) When non-SI units are used they must be adequately explained unless their definition is obvious (*e.g.* degree Celsius, mmHg, g, h). The derivation of derived non-SI units will be indicated.

(*e*) Equations involving electrical quantities should normally be those appropriate for use with SI (rationalized mks) units. If authors wish to use equations suitable for esu or emu the lack of consistency with SI units must be explicitly noted.

(1) *Base units.* The SI base units are given in Table 1.

(2) *Supplementary units.* The SI also includes two 'supplementary' *dimensionless* units as follows:

Physical quantity	Name of unit	Symbol for unit
plane angle	radian	rad
solid angle	steradian	sr

(3) *Multiples and sub-multiples.* In the SI there is one and only one basic unit for each physical quantity. Decimal fractions and multiples of these basic units may, however, be constructed by use of certain prefixes (see Table 2). They may also be used with derived SI units.

The combination of a prefix and a unit symbol constitutes a new single unit symbol; compounding of prefixes is not permitted.

Although it will not always be possible, particularly in Tables, the general principle should be to choose a unit (*i.e.* including multiple or sub-multiple) such that the resulting numerical value is between 0.1 and 1 000.

(4) *Derived units.* Some derived units have special names and symbols and these are given in Table 3. Others do not (Table 4).

(5) *Symbol.* The symbol for a unit will be printed in roman (upright) type, remains unaltered in the plural and does *not* take a full point, *i.e.* 5 cm (not 5 cm. or 5 cms or 5 cms.).

The symbol will be separated from the numerical value by a thin space.

(6) *Decimal fractions and multiples of SI units having special names.* These names are not part of the SI, but for the time being their use in the Society's publications may continue. The list given in Table 5 is not exhaustive.

(7) *Units defined in terms of the best available experimental values of certain physical constants.* These units are not part of the SI. The factors for conversion of these units into SI units are subject to change in the light of new experimental measurements of the constants involved. Their use outside the restricted

Table 1 Base units

Physical quantity	Name of base unit	Symbol for unit
length	metre	m
mass	kilogram	kg
time	second	s
electrical current	ampere	A
thermodynamic temperature	kelvin	K
luminous intensity	candela	cd
amount of substance	mole	mol

Table 2 Prefixes

Fraction	Prefix	Symbol	Multiple	Prefix	Symbol
10^{-1}	deci	d	10	deca	da
10^{-2}	centi	c	10^2	hecto	h
10^{-3}	milli	m	10^3	kilo	k
10^{-6}	micro	μ	10^6	mega	M
10^{-9}	nano	n	10^9	giga	G
10^{-12}	pico	p	10^{12}	tera	T
10^{-15}	femto	f			
10^{-18}	atto	a			

Table 3 Derived units with special names and symbols

Physical quantity	Name of SI unit	Symbol for SI unit	Definition of SI unit
energy	joule	J	$\mathrm{kg\,m^2\,s^{-2}}$
force	newton	N	$\mathrm{kg\,m\,s^{-2} = J\,m^{-1}}$
power	watt	W	$\mathrm{kg\,m^2\,s^{-3} = J\,s^{-1}}$
electric charge	coulomb	C	$\mathrm{A\,s}$
electric potential difference	volt	V	$\mathrm{kg\,m^2\,s^{-3}\,A^{-1} = J\,A^{-1}\,s^{-1}}$
electric resistance	ohm	Ω	$\mathrm{kg\,m^2\,s^{-3}\,A^{-2} = V\,A^{-1}}$
electric capacitance	farad	F	$\mathrm{A^2\,s^4\,kg^{-1}\,m^{-2} = A\,s\,V^{-1}}$
magnetic flux	weber	Wb	$\mathrm{kg\,m^2\,s^{-2}\,A^{-1} = V\,s}$
inductance	henry	H	$\mathrm{kg\,m^2\,s^{-2}\,A^{-2} = V\,A^{-1}\,s}$
magnetic flux density	tesla	T	$\mathrm{kg\,s^{-2}\,A^{-1} = V\,s\,m^{-1}}$
luminous flux	lumen	lm	$\mathrm{cd\,sr}$
illumination	lux	lx	$\mathrm{cd\,sr\,m^{-2}}$
frequency	hertz	Hz	$\mathrm{s^{-1}}$

contexts to which they are appropriate should be discouraged. The following list is not exhaustive.

Physical quantity	Name of unit	Symbol for unit	Conversion factor
energy	electronvolt	eV	$\mathrm{eV} = 1.602\,18 \times 10^{-19}\,\mathrm{J}$
mass	unified atomic mass unit	u	$\mathrm{u} = 1.660\,54 \times 10^{-27}\,\mathrm{kg}$

(8) *Other units now exactly defined in terms of the SI units.* These units are not part of the SI. It is recognized that their use may be continued for some time but it is recommended that except in special circumstances they should be progressively abandoned in conformity with international recommendations. The list given in Table 6 is by no means exhaustive. Each of the definitions given in the fourth column is *exact*.

4.10 Notes for Typists

Manuscripts must be typed in double-line spacing, single sided on A4 paper, with margins at top, bottom and left-hand side of at least 4 cm.

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

(i) Name and address for proofs.

(ii) Title of paper, with capitals for first letter of each noun or adjective only.

(iii) Authors' names; an asterisk should follow the name of the author who is to receive any correspondence.

(iv) The address where the work was carried out; if this is different from the present address of the asterisked author, a footnote indicating this present address should be included. Present addresses of other authors are not normally given.

(v) Summary, preceded and followed by a horizontal line, and typed in double-line spacing.

(vi) Main text.

Tables and captions for Figures should be typed on separate sheets at the end of the manuscript.

For typing of headings see section 4.3.5.

No underlining (for italics) is called for, as this will be done by the editor.

5.0 Deposition of Data: Supplementary Publications Scheme

Table 4 Derived units with no special names or symbols

Physical quantity	SI unit	Symbol for SI unit
area	square metre	$\mathrm{m^2}$
volume	cubic metre	$\mathrm{m^3}$
density	kilogram per cubic metre	$\mathrm{kg\,m^{-3}}$
velocity	metre per second	$\mathrm{m\,s^{-1}}$
angular velocity	radian per second	$\mathrm{rad\,s^{-1}}$
acceleration	metre per second squared	$\mathrm{m\,s^{-2}}$
pressure	newton per square metre	$\mathrm{N\,m^{-2}}$
kinematic viscosity, diffusion coefficient	square metre per second	$\mathrm{m^2\,s^{-1}}$
dynamic viscosity	newton second per square metre	$\mathrm{N\,s\,m^{-2}}$
electric field strength	volt per metre	$\mathrm{V\,m^{-1}}$
magnetic field strength	ampere per metre	$\mathrm{A\,m^{-1}}$
luminance	candela per square metre	$\mathrm{cd\,m^{-2}}$

Bulk information (such as primary kinetic data, computer programs and output, evidence for amino-acid sequences, spectra, *etc.*), which accompanies papers published in the *Journal of the Chemical Society* may be deposited, free of charge, with the Society's Supplementary Publications Scheme, 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.

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 the supplementary material will be sent by the Society to the British Library Document Supply Centre (Boston Spa) (BLDSC), where it will be stored. Copies will be obtainable by individuals both in the UK and abroad on quoting a supplementary publication number that will appear in the parent article.

5.1 Preparation of Material

Authors will be responsible for the preparation of camera-ready copy according to the following specifications (although the Society will be prepared to help in case of difficulty).

(*a*) Optimum page size for text or tables in typescript: up to 30 cm × 21 cm.

(*b*) Limiting page size for text or tables in typescript: 33 cm × 24 cm.

(*c*) Limiting size for diagrams, graphs, spectra, *etc.*: 39 cm × 28.5 cm.

(*d*) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.

(*e*) Pages should be clearly numbered.

It is recommended that all material which is to be deposited should be accompanied by some prefatory text. Normally this will be the summary from the parent paper and authors will greatly aid the deposition of the material if a duplicate copy of the summary is provided.

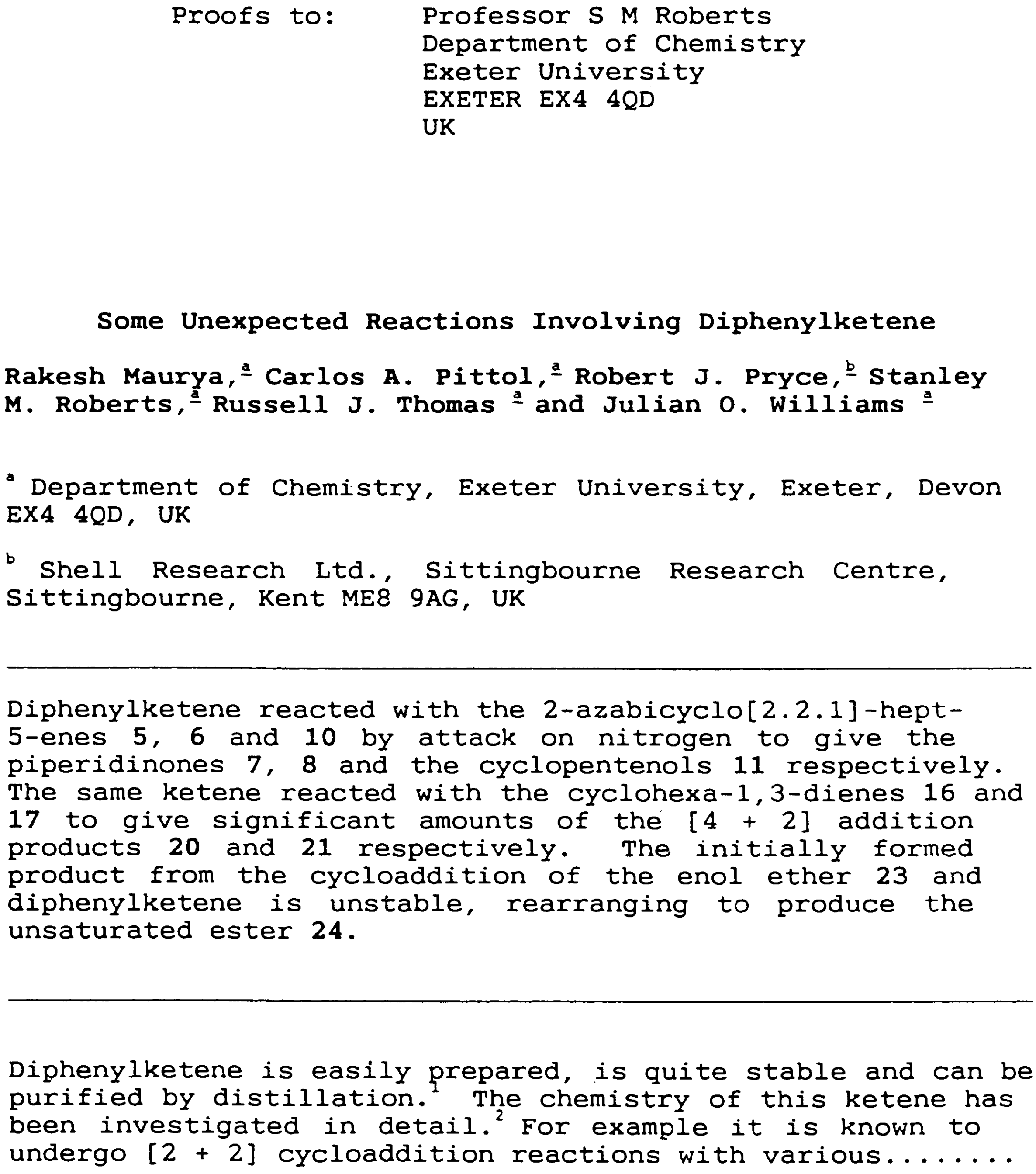
5.2 Deposition

The Society will be responsible for the deposition of the material with the BLDSC. The BLDSC will not receive material direct from authors since the Library wishes to ensure that the material has been properly and adequately refereed.

5.3 Action by the Society

The Society will receive a manuscript for publication together with any supplementary material for deposition and will circulate all this to referees in the normal way. When the edited manuscript is sent to the printers the supplementary material will be sent for deposition to the BLDSC. The Society will add to the paper a footnote indicating what material has been

Specimen first page of typescript



Proofs to: Professor S M Roberts
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Exeter University
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UK

Some Unexpected Reactions Involving Diphenylketene

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Diphenylketene reacted with the 2-azabicyclo[2.2.1]-hept-5-enes **5**, **6** and **10** by attack on nitrogen to give the piperidinones **7**, **8** and the cyclopentenols **11** respectively. The same ketene reacted with the cyclohexa-1,3-dienes **16** and **17** to give significant amounts of the [4 + 2] addition products **20** and **21** respectively. The initially formed product from the cycloaddition of the enol ether **23** and diphenylketene is unstable, rearranging to produce the unsaturated ester **24**.

Diphenylketene is easily prepared, is quite stable and can be purified by distillation.[1] The chemistry of this ketene has been investigated in detail.[2] For example it is known to undergo [2 + 2] cycloaddition reactions with various........

deposited in the Supplementary Publications Scheme and the supplementary publication number.

5.4 Availability

Copies of Supplementary Publications may be obtained from the BLDSC on demand by organizations which are registered borrowers. They should use the normal forms and coupons for such requests addressing them as follows:

Customer Services,
British Library Document Supply Centre,
Boston Spa,
Wetherby,
West Yorkshire, LS23 7BQ, UK

Non-registered users may also obtain copies of Supplementary Publications but should first apply for price quotations. These are available from the Loans Office at the above address.

6.0 Publication of X-Ray Crystallographic Work

Crystallographic work will be assessed mainly for its chemical interest. Thus crystallographic work carried out as part of a wider chemical study should not normally be submitted for publication separately from the results of that study. However, papers reporting only the results of crystal structure determinations may be accepted for publication provided that these results are considered to possess specifically chemical significance.

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 a paper (or at the end of the Experimental section, if this precedes the Discussion). If the procedures for data collection and structure analysis were routine, their description should be particularly concise.

6.1 Summary

The summary of a paper reporting a crystallographic structure determination should normally contain the words 'Crystal Structure of . . .' It need not contain cell dimensions and other crystal data, but should make clear that a crystal structure analysis has been performed.

6.2 Presentation of Crystal Data

The following sequence should be employed (although not all items will be required in all cases): (1) chemical formula and formula weight (M); (2) crystal system; (3) unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, method of determination and temperature (if not ambient); (4) type and wavelength of radiation used; (5) space-group symbol (if non-standard give related standard setting); (6) measured density (D_m), No. of molecules in unit cell (Z), and calculated density (D_x) (with any implications for 'molecular symmetry'); (7) colour, size, and shape of crystal used for data collection; (8) linear absorption coefficient (μ).

Table 5 Fractions and multiples of units with special names

Physical quantity	Name of unit	Symbol for unit	Definition of unit
length	ångström	Å	10^{-10} m = 10^{-1} nm
length	micron	µm	10^{-6} m
area	barn	b	10^{-28} m^2
volume	litre	l	10^{-3} m^3 = dm^3
mass	tonne	t	10^3 kg = Mg
force	dyne	dyn	10^{-5} N
pressure	bar	bar	10^5 N m^{-2}
pressure	pascal	Pa	N m^{-2}
energy	erg	erg	10^{-7} J
kinematic viscosity, diffusion coefficient	stokes	St	10^{-4} m^2 s^{-1}
dynamic viscosity	poise	P	10^{-1} kg m^{-1} s^{-1}
magnetic flux	maxwell	Mx	10^{-8} Wb
magnetic flux density (magnetic induction)	gauss	G	10^{-4} T
conductance	siemens	S	Ω^{-1}

6.3 Data Collection and Processing

The description of data collection should contain sufficient information for the reliability of the determination to be assessed. The following should normally be included.

(1) Type of diffractometer, measuring mode and temperature if not ambient (with reference if possible to an earlier full description).

(2) Theta range and reciprocal lattice segment.

(3) Number of data measured, number observed, and $I/\sigma(I)$ criterion used (if more than one asymmetric unit is recorded, the merging R value should be given).

(4) Absorption correction and method used (with reference).

(5) Stability of intensity controls and any action taken.

6.4 Structure Analysis and Refinement

The information provided should fulfil the same criteria as for data collection (section 6.3). This would normally include:

(1) Method of solution (direct, heavy atom, or combination) and development.

(2) Mode of refinement (full matrix, blocked, block diagonal, anisotropic, isotropic, or mixed), treatment of hydrogen atoms, and weighting scheme.

(3) Final values of R and R_w (and their definitions), with a statement of whether unobserved reflections were included (and if so, how) and if possible some estimate of the accuracy of the F_o data.

(4) Programs or packages and computers used (with references) and source of f data (also f', f'').

(5) Range of standard deviations for bond lengths and angles.

(6) Any procedures used for definition of chirality (quotation of a single Hamilton ratio without specifying the R values from which the ratio was derived and the conditions under which these were obtained, will not normally be acceptable).

When the analysis has not been of a routine nature, authors should explain concisely all procedures used.

6.5 Example of Presentation

The following example demonstrates the application of the recommendations in the preceding sections (6.2 to 6.4):

Experimental

Crystals were prepared as described in ref. 11 and sealed under nitrogen in Lindemann capillaries.

Table 6 Units defined in terms of SI units

Physical quantity	Name of unit	Symbol for unit	Definition of unit
length	inch	in	2.54 × 10^{-2} m
mass	pound (avoirdupois)	lb	0.453 592 37 kg
time*	minute	min	60 s
time*	hour	h	3600 s
force	kilogram-force	kgf	9.806 65 N
force	pound-force	lbf	9.806 65 × 0.453 592 37 N
pressure	atmosphere	atm	101 325 N m^2
pressure	conventional millimetre of mercury	mmHg	13.5951 × 9.806 65 N m^{-2}
pressure	torr	Torr	(101 325/760) N m^{-2}
pressure	pound-force per square inch	lbf in^{-2}	$\frac{9.806\,65 + 4\,535.9237}{6.4516}$ N m^{-2}
energy	kilowatt hour	kW h	3.6 × 10^4 J
energy	thermochemical calorie	cal(thermochem.)	4.184 J
energy	international calorie	cal_{IT}	4.1868 J
thermodynamic temperature	degree Rankine	°R	(5/9) K
radioactivity	curie	Ci	3.7 × 10^{16} s^{-1}

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* Use of other common units (min, h, day) may continue in normal expressions of intervals of time.

Crystal data

$C_{24}H_{26}Cl_3Re_3Si_6$, $M = 1\,028.0$. Monoclinic, $a = 12.021(3)$, $b = 20.489(5)$, $c = 18.194(5)$ Å, $\beta = 91.03(3)°$, $V = 4\,480$ Å^3 (by least-squares refinement on diffractometer angles for 15 automatically centred reflections, $\lambda = 0.710\,69$ Å), space group $P2_1/n$ (alt. $P2_1/c$, No. 14), $Z = 4$, $D_x = 1.76$ g cm^{-3}. Dark blue, air-sensitive tablets. Crystal dimensions (distance to faces from centre): 0.313($211,\bar{2}\bar{1}\bar{1}$) × 0.163($010,\bar{0}\bar{1}\bar{0}$) × 0.063($101,\bar{1}\bar{0}\bar{1}$) mm, μ(Mo-Kα) = 85.12 cm^{-1}.

Data collection and processing[12]

CAD4 diffractometer, $\omega/2\theta$ mode with ω scan width = 0.85 + 0.35 tan θ, ω scan speed 1.3–6.8 deg min^{-1}, graphite-monochromated Mo-Kα radiation; 6383 reflections measured ($1.5 \leqslant \theta \leqslant 25°$, $+h,k,l$), 5797 unique [merging $R = 0.024$ after absorption correction (max., min. transmission factors = 0.37, 0.10)], giving 4 170 with $I > 2\sigma(I)$. Linear and approx. isotropic crystal decay, *ca.* 37% corrected during processing.

Structure analysis and refinement

Direct methods (Re and Cl atoms) followed by normal heavy-atom procedures. Full-matrix least-squares refinement (in two blocks for final, anisotropic cycles) with all non-hydrogen atoms anisotropic and hydrogens in calculated positions with one, overall, refined μ_{iso} [$= 0.08(2) \Rightarrow^2$]. The weighting scheme $w = 1/[\sigma^2(F_o) + 0.0078F_o{}^2]$, with $\sigma(F_o)$ from counting statistics[12] gave satisfactory agreement analyses. Final R and R_w values are 0.062, 0.064. Programs and computers used and sources of scattering factor data are given in ref. 12.

References

11 Ref. to prep. of compound.
12 For full details of experimental techniques used see ref. to previous paper giving full details of data collection procedures *etc.* used in author's laboratory.

6.6 Presentation of Tables and Diagrams

A clear distinction should be made between material to appear in print and material for deposition.

6.6.1 *For Publication in the Journal.*—Only important **selected** bond lengths/angles will be published. These should be presented in the manuscript, with full details in the supplementary data for referees and/or deposition. A conventional *line drawing* of the structure must 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 system* 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}).

6.6.2 *For the Referees and/or for Deposition.*—(1) A table of final fractional atomic coordinates (labelled x, y, z).

(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 *thermal parameters* in the form B_{ij} or U_{ij} (in Å^2 or pm^2).

(5) Details of any *least-squares planes* used to provide parameters for the paper.

(6) A legible table of *structure factors* (F_o, F_c) (for the referees only; not for deposition).*

6.6.3 *Deposition of Material at the Cambridge Crystallographic Data Centre.*—The table of final *fractional atomic coordinates,* the full list of *bond lengths and angles* and the list of *thermal parameters* will be deposited at the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ (or at the *Fachinformationszentrum* Karlsruhe, D-7514, Eggenstein-Leopoldshafen 2, *via* Dr P. Luksch, for molecules not containing 'organic' carbon). The material for deposition should include a completed abstract form for each crystallographic determination (a blank for photocopying is reproduced at the end of these instructions). All tables should be of publication 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 *Fachinformationszentrum* Karlsruhe for deposited material should be accompanied by the full literature citation for the paper concerned.

As an alternative to the printed material, authors are encouraged to supply data for the Cambridge 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.

6.7 Reference to Crystallographic Work Published in Preliminary Form

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

6.8 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 the referees 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 referee to make sure that the point made is correct, and coordinates *etc.* will be deposited at the Cambridge

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* Authors should preserve copies of structure factor tables in their own records.

Crystallographic Data Centre (or *Fachinformationszentrum* Karlsruhe). The brief published description of the determination should be supplemented by appropriate reference to 'unpublished work'.

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 *Faraday Transactions*, one in which the computations are incidental to the chemistry to *Perkin*, *Dalton*, or *Faraday Transactions*. Papers concerned mainly with computational details are unlikely to be accepted.

(*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 with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

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 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 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, algorithmic options, *etc.* 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

The *Perkin* Editorial Board are concerned that natural product structure elucidation papers should be accepted for publication in the *Journal* 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 Guidelines for Submission on Disk

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Characters – note distinction between ell (l) and one (1) and upper case oh (O) and zero (0)

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CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM

Compound Name

Diagram *(conventional chemical structural diagram)*

Formula *(each residue to be formulated ,eg.* $C_2H_3O_2^{-}\cdot Na^{+}\cdot 2H_2O$*)*

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)*

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APPENDIX

IUPAC Publications on Nomenclature and Symbolism

1.0 Compilations

1.1 Nomenclature of Organic Chemistry, a 550-page hardcover volume published in 1979, available from Pergamon, Oxford.

Section A: Hydrocarbons
Section B: Fundamental heterocyclic systems
Section C: Characteristic groups containing carbon, hydrogen, oxygen, nitrogen, halogen, sulfur, selenium and tellurium
Section D: Organic compounds containing elements not exclusively those referred to in the title of Section C
Section E: Stereochemistry
Section F: General principles for the naming of natural products and related compounds
Section H: Isotopically modified compounds

1.2 A Guide to IUPAC Nomenclature of Organic Compounds, a 182-page softcover volume published in 1993, available from Blackwell Scientific Publications, Oxford, to be used in conjunction with item 1.1.

1.3 Nomenclature of Inorganic Chemistry, a 278-page hardcover volume published in 1990, available from Blackwell Scientific Publications, Oxford.

Chapter 1: General aims, functions and methods
Chapter 2: Grammar
Chapter 3: Elements, atoms and groups
Chapter 4: Formulae
Chapter 5: Names based on stoichiometry
Chapter 6: Neutral molecular compounds
Chapter 7: Names for ions, substituent groups and radicals, and salts
Chapter 8: Oxoacids and derived anions
Chapter 9: Co-ordination compounds
Chapter 10: Boron hydrides and related compounds

1.4 Biochemical Nomenclature and Related Documents, a 348-page softcover manual published in 1992 by Portland Press Ltd. for IUBMB, and available from the publisher (59 Portland Place, London W1N 3AJ, UK). The contents are as follows:

Nomenclature of organic chemistry. Section E: Stereochemistry (1974)
Nomenclature of organic chemistry. Section F: Natural products and related compounds (1976)
Isotopically modified compounds
Recommendations for the presentation of thermodynamic and related data in biology (1985)
Citation of bibliographic references in biochemical journals (1971)
Nomenclature and symbolism for amino acids and peptides (1983)
Abbreviated nomenclature of synthetic polypeptides or polymerized amino acids (1971)
Abbreviations and symbols for the description of the conformation of polypeptide chains (1969)
Nomenclature of peptide hormones (1974)
Nomenclature of glycoproteins, glycopeptides and peptidoglycans (1985)
Nomenclature of initiation, elongation and termination factors for translation in eukaryotes (1988)
Nomenclature of multiple forms of enzymes (1976)
Symbolism and terminology in enzyme kinetics (1981)
Nomenclature for multienzymes (1989)
Abbreviations and symbols for nucleic acids, polynucleotides and their constituents (1970)
Abbreviations and symbols for the description of the conformations of polynucleotide chains (1982)
Nomenclature for incompletely specified bases in nucleic acid sequences (1984)
Carbohydrate nomenclature. Part I (1969)
Nomenclature of cyclitols (1973)
Numbering of atoms in *myo*-inositol (1988)
Conformational nomenclature for five- and six-membered ring forms of monosaccharides and their derivatives (1980)
Nomenclature of unsaturated monosaccharides (1980)
Nomenclature of branched-chain monosaccharides (1980)
Abbreviated terminology of oligosaccharide chains (1980)
Polysaccharide nomenclature (1980)
Symbols for specifying the conformation of polysaccharide chains (1981)
Nomenclature of lipids (1976)
Nomenclature of steroids (1989)
Nomenclature of quinones with isoprenoid side chains (1973)
Nomenclature of carotenoids (1970) and amendments (1974)
Nomenclature of tocopherols and related compounds (1981)
Nomenclature of vitamin D (1981)
Nomenclature of retinoids (1981)
Prenol nomenclature (1986)
Nomenclature of phosphorus-containing compounds of biochemical importance (1976)
Nomenclature and symbols for folic acids and related compounds (1986)
Nomenclature for vitamins B-6 and related compounds (1973)
Nomenclature of corrinoids (1973)
Nomenclature of tetrapyrroles (1986)

1.5 Compendium of Analytical Nomenclature, a 280-page hardcover volume published in 1987, available from Blackwell Scientific Publications, Oxford. The contents are as follows:

Presentation of the Results of Chemical Analysis
Solution Thermodynamics (activity coefficients, equilibria, pH)
Recommendations for Terminology to be used with Precision Balances
Recommendations for Nomenclature of Thermal Analysis
Recommendations for Nomenclature of Titrimetric Analysis
Electrochemical Analysis
Analytical Separation Processes (precipitation, liquid-liquid distribution, zone melting and fractional crystallisation, chromatography, ion exchange)
Spectrochemical Analysis (radiation sources, general atomic emission spectroscopy, flame spectroscopy, X-ray emission spectroscopy, molecular methods)
Recommendations for Nomenclature of Mass Spectrometry
Recommendations for Nomenclature of Radiochemical Methods
Surface Analysis (including photoelectron spectroscopy)

1.6 Compendium of Macromolecular Nomenclature, a 172-page hardcover volume published in 1991, available from Blackwell Scientific Publications, Oxford. The contents are as follows:

Basic Definitions of Terms Relating to Polymers
Stereochemical Definitions and Notations Relating to Polymers
Definitions of Terms Relating to Individual Macromolecules, their Assemblies, and Dilute Polymer Solutions
Definitions of Terms Relating to Crystalline Polymers
Nomenclature of Regular Single-strand Organic Polymers
Nomenclature for Regular Single-strand and Quasi-single-strand Inorganic and Coordination Polymers
Source-based Nomenclature for Copolymers
A Classification of Linear Single-strand Polymers
Use of Abbreviations for Names of Polymeric Substances

1.7 Compendium of Chemical Terminology: IUPAC Recommendations, a 456-page volume published in 1987, available in hardcover and softcover from Blackwell Scientific Publications, Oxford.

1.8 Quantities, Units and Symbols in Physical Chemistry, a 166-page softcover volume published in 1993 by Blackwell Scientific Publications, Oxford.

2.0 Documents not included in the compilations

2.1 Nomenclature of Elements and Compounds

Boron Compounds

Nomenclature of inorganic boron compounds (*Pure Appl. Chem.*, 1972, **30**, 681).

Carbon

Nomenclature and terminology of graphite intercalation compounds (*Pure Appl. Chem.*, 1994, **66**, 1893).

Recommended terminology for the description of carbon as a solid (*Pure Appl. Chem.*, 1995, **67**, 473).

Class Names

Glossary of class names of organic compounds and reactive intermediates based on structure (*Pure Appl. Chem.*, 1995, **67**, 1307).

Delta Convention

Nomenclature for cyclic organic compounds with contiguous formal double bonds (*Pure Appl. Chem.*, 1988, **60**, 1395).

Elements

Names and symbols of transfermium elements (*Pure Appl. Chem.*, 1994, **66**, 2419).

Enzymes

Enzyme Nomenclature (1992), published by Academic Press in hardcover and softcover editions.

Heterocyclic Compounds

Revision of the extended Hantzsch-Widman system of nomenclature for heteromonocycles (*Pure Appl. Chem.*, 1983, **55**, 409).

Hydrogen

Names for hydrogen atoms, ions and groups, and for reactions involving them (*Pure Appl. Chem.*, 1988, **60**, 1115).

Isotopically Modified Compounds

Nomenclature of inorganic chemistry. Part II. 1. Isotopically modified compounds (*Pure Appl. Chem.*, 1981, **53**, 1887).

Lambda Convention

Treatment of variable valence in organic nomenclature (*Pure Appl. Chem.*, 1984, **56**, 769).

Nitrogen Hydrides

Nomenclature of hydrides of nitrogen and derived cations, anions and ligands (*Pure Appl. Chem.*, 1982, **54**, 2545).

Numerical Terms

Extension of Rules A-1.1 and A-2.5 concerning numerical terms used in organic chemical nomenclature (*Pure Appl. Chem.*, 1986, **58**, 1693).

Polyanions

Nomenclature of polyanions (*Pure Appl. Chem.*, 1987, **59**, 1529).

Polymers

Nomenclature of regular double-strand (ladder and spiro) organic polymers (*Pure Appl. Chem.*, 1993, **65**, 1561).

Structure-based nomenclature for irregular single-strand organic polymers (*Pure Appl. Chem.*, 1994, **66**, 873).

Graphic representations (chemical formulae) of macromolecules (*Pure Appl. Chem.*, 1994, **66**, 2469).

Basic classification and definitions of polymerization reactions (*Pure Appl. Chem.*, 1994, **66**, 2483).

Radicals and Ions

Revised nomenclature for radicals, ions, radical ions and related species (*Pure Appl. Chem.*, 1993, **65**, 1357).

Zeolites

Chemical nomenclature and formulation of compositions of synthetic and natural zeolites (*Pure Appl. Chem.*, 1979, **51**, 1091).

2.2 Terminology, Symbols and Units, and Presentation of Results

General

Glossary of terms used in physical organic chemistry (*Pure Appl. Chem.*, 1994, **66**, 1077).

Glossary of atmospheric chemistry terms (*Pure Appl. Chem.*, 1990, **62**, 2167).

Units for use in atmospheric chemistry (*Pure Appl. Chem.*, 1995, **67**, 1377).

English-derived abbreviations for experimental techniques in surface science and chemical spectroscopy (*Pure Appl. Chem.*, 1991, **63**, 887).

Analytical

Recommendations for publication of papers on a new analytical method based on ion exchange or ion-exchange chromatography (*Pure Appl. Chem.*, 1980, **52**, 2555).

Recommendations for presentation of data on compleximetric indicators, 1. General (*Pure Appl. Chem.*, 1979, **51**, 1357).

Recommendations for publishing manuscripts on ion-selective electrodes (*Pure Appl. Chem.*, 1981, **53**, 1907).

Recommendations on use of the term amplification reactions (*Pure Appl. Chem.*, 1982, **54**, 2553).

Recommendations for the usage of selective, selectivity and related terms in analytical chemistry (*Pure Appl. Chem.*, 1983, **55**, 553).

Nomenclature for automated and mechanised analysis (*Pure Appl. Chem.*, 1989, **61**, 1657).

Nomenclature for sampling in analytical chemistry (*Pure Appl. Chem.*, 1990, **62**, 1193).

Nomenclature for chromatography (*Pure Appl. Chem.*, 1993, **65**, 819).

Nomenclature of kinetic methods of analysis (*Pure Appl. Chem.*, 1993, **65**, 2291).

Nomenclature for liquid–liquid distribution (solvent extraction) (*Pure Appl. Chem.*, 1993, **65**, 2373).

Nomenclature for supercritical fluid chromatography and extraction (*Pure Appl. Chem.*, 1993, **65**, 2397).

Nomenclature and terminology for analytical pyrolysis (*Pure Appl. Chem.*, 1993, **65**, 2405).

Nomenclature for the presentation of results of chemical analysis (*Pure Appl. Chem.*, 1994, **66**, 595).

Recommendations for nomenclature in laboratory robotics and automation (*Pure Appl. Chem.*, 1994, **66**, 609).

Nomenclature of interlaboratory analytical studies (*Pure Appl. Chem.*, 1994, **66**, 1903).

Nomenclature of thermometric and enthalpimetric methods in chemical analysis (*Pure Appl. Chem.*, 1994, **66**, 2487).

Classification and definition of analytical methods based on flowing media (*Pure Appl. Chem.*, 1994, **66**, 2493).

Nomenclature for radioanalytical chemistry (*Pure Appl. Chem.*, 1994, **66**, 2513).

Glossary of bioanalytical nomenclature—Part 1: General terminology, body fluids, enzymology, immunology (*Pure Appl. Chem.*, 1994, **66**, 2587).

Biotechnology

Glossary for chemists of terms used in biotechnology (*Pure Appl. Chem.*, 1992, **64**, 143).

Selection of terms, symbols and units related to microbial processes (*Pure Appl. Chem.*, 1992, **64**, 1047).

Clinical

Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (*Pure Appl. Chem.*, 1984, **56**, 567).

Quantities and units in clinical chemistry (*Pure Appl. Chem.*, 1979, **51**, 2451).

Quantities and units in clinical chemistry: nebulizer and flame properties in flame emission and absorption spectrometry (*Pure Appl. Chem.*, 1986, **58**, 1737).

List of quantities in clinical chemistry (*Pure Appl. Chem.*, 1979, **51**, 2481).

Proposals for the description and measurement of carry-over effects in clinical chemistry (*Pure Appl. Chem.*, 1991, **63**, 301).

Quantities and units for metabolic processes as a function of time (*Pure Appl. Chem.*, 1992, **64**, 1569).

Quantities and units for electrophoresis in the clinical laboratory (*Pure Appl. Chem.*, 1994, **66**, 891).

Quantities and units for centrifugation in the clinical laboratory (*Pure Appl. Chem.*, 1994, **66**, 897).

Colloids and Surface Chemistry

Definitions, terminology and symbols in colloid and surface chemistry. I (*Pure Appl. Chem.*, 1972, **31**, 577). II, Heterogeneous catalysis (*Pure Appl. Chem.*, 1976, **46**, 71). Part 1.14: Light scattering (provisional) (*Pure Appl. Chem.*, 1983, **55**, 931).

Reporting experimental pressure–area data with film balances (*Pure Appl. Chem.*, 1985, **57**, 621).

Reporting physisorption data for gas/solid systems with special reference to the determination of surface area and porosity (*Pure Appl. Chem.*, 1985, **57**, 603).

Reporting data on adsorption from solution at the solid/solution interface (*Pure Appl. Chem.*, 1986, **58**, 967).

Manual on catalyst characterization (*Pure Appl. Chem.*, 1991, **63**, 1227).

Thin films including layers: terminology in relation to their preparation and characterization (*Pure Appl. Chem.*, 1994, **66**, 1667).

Electrochemistry

Nomenclature for transfer phenomena in electrolytic systems (*Pure Appl. Chem.*, 1981, **53**, 1827).

Electrode reaction orders, transfer coefficients and rate constants—amplification of definitions and recommendations for publication of parameters (*Pure Appl. Chem.*, 1980, **52**, 233).

Classification and nomenclature of electroanalytical techniques (*Pure Appl. Chem.*, 1976, **45**, 81).

Recommendations for sign conventions and plotting of electrochemical data (*Pure Appl. Chem.*, 1976, **45**, 131).

Electrochemical nomenclature (*Pure Appl. Chem.*, 1974, **37**, 499).

Recommendations on reporting electrode potentials in nonaqueous solvents (*Pure Appl. Chem.*, 1984, **56**, 461).

Definition of pH scales, standard reference values, measurement of pH and related terminology (*Pure Appl. Chem.*, 1985, **57**, 531).

Interphases in systems of conducting phases (*Pure Appl. Chem.*, 1986, **58**, 437).

The absolute electrode potential: an explanatory note (*Pure Appl. Chem.*, 1986, **58**, 955).

Electrochemical corrosion nomenclature (*Pure Appl. Chem.*, 1989, **61**, 19).

Terminology in semiconductor electrochemistry and photoelectrochemical energy conversion (*Pure Appl. Chem.*, 1991, **63**, 569).

Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (*Pure Appl. Chem.*, 1991, **63**, 895).

Nomenclature, symbols and definitions in electrochemical engineering (*Pure Appl. Chem.*, 1993, **65**, 1009).

Terminology and conventions for microelectronic ion-selective field effect transistor devices in electrochemistry (*Pure Appl. Chem.*, 1994, **66**, 565).

Impedances of electrochemical systems: terminology, nomenclature and representation—Part 1: Cells with metal electrodes and liquid solutions (*Pure Appl. Chem.*, 1994, **66**, 1831).

Terminology and notations for multistep electrochemical reaction mechanisms (*Pure Appl. Chem.*, 1994, **66**, 2445).

Recommendations for nomenclature of ion-selective electrodes (*Pure Appl. Chem.*, 1994, **66**, 2527).

Kinetics

Symbolism and terminology in chemical kinetics (provisional) (*Pure Appl. Chem.*, 1981, **53**, 753).

Kinetics of composite reactions in closed and open flow systems (*Pure Appl. Chem.*, 1993, **65**, 2641).

Photochemistry

Recommended standards for reporting photochemical data (*Pure Appl. Chem.*, 1984, **56**, 939).

Glossary of terms used in photochemistry (*Pure Appl. Chem.*, 1988, **60**, 1055).

Quantum Chemistry

Expression of results in quantum chemistry (*Pure Appl. Chem.*, 1978, **50**, 75).

Reactions

Nomenclature for organic chemical transformations (*Pure Appl. Chem.*, 1989, **61**, 725).

System for symbolic representation of reaction mechanisms (*Pure Appl. Chem.*, 1989, **61**, 23).

Detailed linear representation of reaction mechanisms (*Pure Appl. Chem.*, 1989, **61**, 57).

Rheological Properties

Selected definitions, terminology and symbols for rheological properties (*Pure Appl. Chem.*, 1979, **51**, 1215).

Spectroscopy

Recommendations for publication of papers on methods of molecular absorption spectrophotometry in solution (*Pure Appl. Chem.*, 1978, **50**, 237).

Recommendations for the presentation of infrared absorption spectra in data collections. A, Condensed phases (*Pure Appl. Chem.*, 1978, **50**, 231).

Definition and symbolism of molecular force constants (*Pure Appl. Chem.*, 1978, **50**, 1709).

Nomenclature and conventions for reporting Mössbauer spectroscopic data (*Pure Appl. Chem.*, 1976, **45**, 211).

Recommendations for the presentation of NMR data for publication in chemical journals. A, Proton spectra (*Pure Appl. Chem.*, 1972, **29**, 625). B, Spectra from nuclei other than protons (*Pure Appl. Chem.*, 1976, **45**, 217).

Presentation of Raman spectra in data collections (*Pure Appl. Chem.*, 1981, **53**, 1879).

Names, symbols, definitions and units of quantities in optical spectroscopy (*Pure Appl. Chem.*, 1985, **57**, 105).

A descriptive classification of the electron spectroscopies (*Pure Appl. Chem.*, 1987, **59**, 1343).

Presentation of molecular parameter values for IR and Raman intensity (*Pure Appl. Chem.*, 1988, **60**, 1385).

Recommendations for EPR/ESR nomenclature and conventions for presenting experimental data in publications (*Pure Appl. Chem.*, 1989, **61**, 2195).

Nomenclature, symbols, units and their usage in spectrochemical analysis. VII. Molecular absorption spectroscopy, UV and visible (*Pure Appl. Chem.*, 1988, **60**, 1449); VIII. Nomenclature system for X-ray spectroscopy (*Pure Appl. Chem.*, 1991, **63**, 735); X. Preparation of materials for analytical atomic spectroscopy (*Pure Appl. Chem.*, 1988, **60**, 1461); XII. Terms related to electrothermal atomization (*Pure Appl. Chem.*, 1992, **64**, 253); XIII. Terms related to chemical vapour generation (*Pure Appl. Chem.*, 1992, **64**, 261).

Recommendations for nomenclature and symbolism for mass spectroscopy (*Pure Appl. Chem.*, 1991, **63**, 1541).

Symbols for fine and hyperfine structure parameters (*Pure Appl. Chem.*, 1994, **66**, 571).

Solid State

Definitions of terms relating to phase transitions of the solid state (*Pure Appl. Chem.*, 1994, **66**, 577).

Thermodynamics

A guide to procedures for the publication of thermodynamic data (*Pure Appl. Chem.*, 1972, **39**, 395).

Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (*Pure Appl. Chem.*, 1981, **53**, 1805).

Notation for states and processes; significance of the word 'standard' in chemical thermodynamics and remarks on commonly tabulated forms of thermodynamic functions (*Pure Appl. Chem.*, 1982, **54**, 1239).

Standard quantities in thermodynamics: fugacities, activities and equilibrium constants for pure and mixed phases (*Pure Appl. Chem.*, 1994, **66**, 533).

Recommendations for nomenclature and tables in biochemical thermodynamics (*Pure Appl. Chem.*, 1994, **66**, 1641).

Toxicology

Glossary for chemists of terms used in toxicology (*Pure Appl. Chem.*, 1993, **65**, 2003).