

## Instructions for Authors (1989)

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### CONTENTS

- 1.0 General Policy**
  - 1.1 Conditions governing acceptance
  - 1.2 Submission of articles
- 2.0 Administration and Publication Procedure**
- 3.0 Presentation of Papers**
  - 3.1 Organization of material
  - 3.2 Brevity
  - 3.3 Linguistic and typographical conventions
  - 3.4 Formulae and figures
  - 3.5 Presentation of experimental data
  - 3.6 Authentication of new compounds
  - 3.7 Bibliographic references and footnotes
  - 3.8 Nomenclature
  - 3.9 Units and symbols
  - 3.10 Notes for typists
- 4.0 Deposition of Data: Supplementary Publications Scheme**
  - 4.1 Preparation of material
  - 4.2 Deposition
  - 4.3 Action by the Society
  - 4.4 Availability
- 5.0 Publication of X-Ray Crystallographic Work**
  - 5.1 Title and summary
  - 5.2 Presentation of crystal data
  - 5.3 Data collection and processing
  - 5.4 Structure analysis and refinement
  - 5.5 Example of presentation
  - 5.6 Presentation of tables and diagrams
  - 5.7 Reference to crystallographic work published in *Chemical Communications*
  - 5.8 Reference to unpublished crystallographic work
- 6.0 Perkin Communications**
- 7.0 Publication of Theoretical and Computational Papers**
- Appendix. IUPAC Publications on Nomenclature and Symbolism**

### 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.

The *Journal* is published in six sections, of which five are termed *Transactions*; these are distinguished by their subject matter, as follows:

*Dalton Transactions (Inorganic Chemistry)*. All aspects of the chemistry of inorganic and organometallic compounds, including bioinorganic chemistry and solid-state inorganic chemistry; the applications of physicochemical techniques to the study of their structures, properties, and reactions, including kinetics and mechanism; new or improved experimental techniques and syntheses.

*Faraday Transactions I (Physical Chemistry in Condensed Phases)*. Colloid and interface science, surface science, physicochemistry and chromatographic science, chemisorption and heterogeneous catalysis, zeolites and ion-exchange phenomena. Electrode processes, liquids and solutions: experimental and theoretical. Solid-state chemistry: microstructures and dynamics. Reactions in condensed phases, physical chemistry of macromolecules and polymers. Biophysical chemistry and radiation chemistry.

*Faraday Transactions II (Molecular and Chemical Physics)*. Gas-phase reaction kinetics and dynamics: experimental and theoretical; molecular beam kinetics and spectroscopy. Photochemistry and photophysics, energy transfer and relaxation processes. Laser-induced chemistry. Spectroscopies of molecules, molecular ensembles, and gas-phase complexes. Quantum theory of molecular structure. Statistical mechanics of gaseous molecules and complexes; statistical mechanics and quantum theory of the condensed phase. Computational chemistry; molecular dynamics.

*Perkin Transactions I (Organic Chemistry)*. All aspects of organic and bio-organic chemistry. These include synthetic organic chemistry of all types, organometallic chemistry, chemistry and biosynthesis of natural products, the relationship between molecular structure and biological activity, the chemistry of polymers and biological macromolecules, and medicinal and agricultural chemistry where there is originality in the science.

*Perkin Transactions II (Physical Organic Chemistry)*. Physicochemical aspects of organic, organometallic, and bio-organic chemistry, including kinetic, mechanistic, structural, spectroscopic, and theoretical studies. Such topics include structure-activity relationships and physical aspects of biological processes and of the study of polymers and biological macromolecules.

Authors are requested to indicate, at the time they submit a typescript, the journal for which it is intended. Should this seem unsuitable, the Editor will inform the author.

The sixth section of the *Journal of the Chemical Society is Chemical Communications*, which is intended as a forum for preliminary accounts of original and significant work, in any area of chemistry that is likely to prove of wide general appeal or exceptional specialist interest. Such preliminary reports should be followed up eventually by full papers in other journals (e.g. the five *Transactions*) providing detailed accounts of the work.

### 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* 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 accepted by the Society on the understanding that the authors (a) have obtained any necessary authority for publication, and (b) will, if requested, 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.\*

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\* Attention is drawn to the following extract from the Society's By-Laws:

91. (iii) Every member who submits a paper or other communication with a view to its publication by the Society shall by so doing undertake: (a) that his communication has not been published and that he will not permit its publication before it is accepted or declined by the Society, and (b) that if it is accepted for publication the Society shall thereupon become entitled to an exclusive licence under any copyright therein (which shall include the right to sublicense) and that he will, if then called upon to do so, execute a formal licence to the Society of the said copyright, including the sole right to publish in any form in any language and in any part of the world, the whole or any part of his communication. The Council shall not refuse any reasonable request from an author to reproduce his own work elsewhere in whole or in part.

(iv) The Society shall have the right to retain manuscripts and illustrative drawings sent to the Society for consideration for publication.

(v) The attention of every member who submits any paper or other communication with a view to its publication shall be drawn to paragraph (iii) of this By-Law above, and any person other than a member shall be required to sign an undertaking in the terms set out therein.

### 1.2 Submission of Articles

Typescripts should be addressed to: The Manager, Journals, The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF.

Three copies of the typescript (a top copy and two good quality carbon or Xerox copies) are required. Copies of any related, relevant, unpublished material should also be provided.

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 and editorial staff 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 Office. 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. This decision and relevant comments of the referees are communicated to the author. Differences of opinion are mediated by the Editor, possibly after consultation with further referees, or, in the last resort, by the Editorial Board.

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 when the edited manuscript is sent to the printer. The author receives two copies of proofs, together with the edited manuscript and reprint order form. The Society supplies 50 reprints free of charge, and further copies can be purchased.

One corrected proof *and* the manuscript, the reprint order form, and payment (if any) 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 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 summarised 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). 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 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.

#### 3.1 Organization of Material

3.1.1 *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.<sup>1</sup> 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.

3.1.2 *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.

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

3.1.4 *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.

3.1.5 *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.

3.1.6 *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.

3.1.7 *Bibliographic References*.—These should be given on a separate sheet at the end of the manuscript; for details see section 3.7.

#### 3.2 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 communication.

(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.)

#### 3.3 Linguistic and Typographical Conventions

3.3.1 *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.

3.3.2 *Abbreviations*.—The following common initial letter abbreviations may be used without definition: b.p., c.d., e.s.r., g.l.c., i.r., m.p., n.m.r., o.r.d., t.l.c., u.v., v/v, w/w. Other such abbreviations should be defined at first mention, as should abbreviations for reagents, *etc.*

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

(a) A comma is placed before 'and' or 'or' in a series such as 'oxygen, sulphur, and selenium' or ' $\lambda_{\max}$ , 237, 295, and 343 nm.'

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

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

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

(e) Parenthetical expressions of the same physical quantity in different units are separated by a comma, *e.g.* (3.9 g, 0.1 mol), (30 ml, 1 mol); expressions of different physical quantities are separated by a semicolon, *e.g.* (2.9 g cm<sup>-3</sup>; 30 ml).

3.3.4 *Hyphenation*.—Hyphens are used for two purposes: to divide and to compound.

*Division*. It is common practice to divide words, particularly when in a sequence, when one part is common to several of the words; in such cases, the hyphen, representing the point of attachment to the common part, is always inserted, e.g. 'the chloro-, bromo-, and fluoro-naphthacenes,' 'the *o*-, *m*-, or *p*-nitrotoluenes,' or 'the oxo-naphthalenes and -naphthacenes.' It is not good practice, however, to detach both a common prefix and a common suffix in a series, e.g. 'the dihydroxy-naphthalene- and phenanthrene-diones,' since confusion can arise.

It is customary to separate a pair of the same letter when these letters (in the same fount) would not naturally fall together, e.g. butyl-lithium, iodo-octane.

*Compounding*. A hyphen is often necessary when words are compounded to form a single modifying adjective to precede the noun being modified, thus, 'a melting-point determination' or 'a free-radical chain mechanism.' A hyphen is not needed when adverbs are compounded, as in 'an electrically heated oven,' or for two-word chemical names such as 'nitric acid solution.'

*Miscellaneous uses of hyphens*. Hyphens are used to set apart numbers, configurational letters, Greek letters, and italicized prefixes, e.g. 1,2,5-trimethylcyclohexane, *D*-*gluco*-hexose,  $\beta$ -chlorophenethylbenzene, tri- $\mu$ -carbonyl-bis(tricarbonyliron), and *cis*-decalin.

3.3.5 *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*-hexane-1,2-diol, *gem*- and *vic*-diols, benzil *anti*-oxime, 3-*O*-methyl-*L*-glycero-tetrose.

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

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

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

*Note*: Greek letters are not italicised.

3.3.6 *Headings*.—(a) Main sections (Experimental, Discussion, *etc.*): side-heading, bold, no final fullstop.

(b) Main side-heading: italics, initial capital letter for each noun and adjective, final fullstop and dash.

(c) Subsidiary side-heading: italics, first initial capital only, final fullstop but no dash.

(d) Further subdivision: by italic (*a*), (*b*), *etc.* (no following fullstop), and finally (i), (ii), *etc.* If (*a*), (*b*), *etc.* are used in front of a subsidiary side-heading, then for contrast these letters are not italicized.

Letters and prefixes which are ordinarily printed in italics are transferred for contrast into roman type in italicized phrases (see example below, where *O*-alkyl becomes *O*-alkyl).

Physicochemical symbols, however, remain in their prescribed form, and numerals and Greek letters are not italicized.

*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 . . .

### 3.4 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.

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

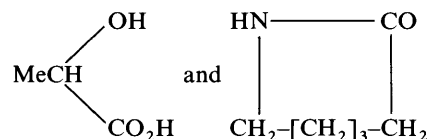
(b) Formulae should be numbered with bold arabic numerals in parentheses [(1), (2), and (3) *etc.*] in the order in which they are displayed and not in the order of mention in text.

(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.

HO-CHMe-CO<sub>2</sub>H and  $\overline{\text{NH}}\text{---}[\text{CH}_2]_5\text{---CO}$  rather than



(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*-HO-C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>-NH<sub>2</sub> and CH<sub>2</sub>Cl-CH(OH)-CO<sub>2</sub>H.

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.

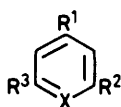
Repeating sequences of a backbone composite group are enclosed in square brackets and their number is indicated by an inferior multiplier, e.g. HO[CH<sub>2</sub>]<sub>4</sub>NH<sub>2</sub>, but HO[CH<sub>2</sub>]<sub>4</sub>N-(CH<sub>2</sub>OH)<sub>2</sub>.

(g) Steric conventions must be observed, notably for steroids, triterpenes, and carbohydrates. The Society uses wedges ( $\blacktriangleleft$ ) or heavy lines ( $\text{---}$ ) rather than blocked circles ( $\bullet$ ), and broken lines in the form  $\text{---}$  or  $\text{|||}$

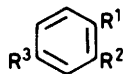
(h) The abbreviations Me, Et, Pr<sup>n</sup>, Pr<sup>i</sup>, Bu<sup>n</sup>, Bu<sup>i</sup>, Bu<sup>s</sup>, Bu<sup>t</sup>, Ph, Ac, Alk, Ar, and Hal, should be used except when the group is involved in the reaction described. Other special symbols, if used, require an explanatory footnote. The carboxy-group is written CO<sub>2</sub>H (not COOH); similarly CO<sub>2</sub>R.

(i) One variable univalent substituent is indicated by R; when more than one independently variable general substituent is present, R<sup>1</sup>, R<sup>2</sup>, and R<sup>3</sup> should be used (not R, R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>; or R<sub>1</sub>, R<sub>2</sub>, and R<sub>3</sub> 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<sup>1</sup> = R<sup>2</sup> = Ph, R<sup>3</sup> = Me, X = O<sup>+</sup>  
 (2) R<sup>1</sup> = Me, R<sup>2</sup> = R<sup>3</sup> = Ph, X = S<sup>+</sup>



- (3) R<sup>1</sup> = Me, R<sup>2</sup> = Ph, R<sup>3</sup> = PhCO  
 (4) R<sup>1</sup>R<sup>2</sup> = CO-O-CO, R<sup>3</sup> = 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.

3.4.2 *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 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*/atm), 10<sup>3</sup>(*T*/K)<sup>-1</sup>.

(g) Captions and explanatory legends to be set by the printer should be typed on a separate page attached to the manuscript, and not given on the figure itself.

(h) Figures are numbered consecutively Figure 1, Figure 2, etc. (in arabic numerals).

(i) 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.

### 3.5 Presentation of Experimental Data

3.5.1 *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.* *p*V<sup>G</sup>, or some mathematical function of such a number, *e.g.* ln(*p*<sup>m</sup>/atm).

*Example:*

θ/°C	<i>T</i> /K	10 <sup>3</sup> K/ <i>T</i>	<i>p</i> /atm	ln( <i>p</i> /atm)	<i>V</i> <sub>m</sub> <sup>G</sup> /cm <sup>3</sup> mol <sup>-1</sup>	<i>pV</i> <sub>m</sub> <sup>G</sup> / <i>RT</i>
-51.60	216.55	4.6179	5.112	1.6316	3 177.6	0.9142

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

If possible, tables should be arranged so as not to require printing sideways on the page ('landscape') unless their depth is such that the page will be filled; otherwise division into two tables is preferred.

3.5.2 *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, u.v. absorptions, i.r. absorptions, n.m.r. 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 'm.p. 75 °C (from EtOH), i.e. the crystallisation solvent in parentheses. If an identical mixed melting point is to be recorded, the form 'm.p. and mixed m.p. 75 °C' is appropriate.

**Optical rotation.** Shown in the form  $[\alpha]_D^{22} -22.5^\circ$  (*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, a distinction is made between 'new' and 'known' compounds (see section 3.6).

New compounds should be indicated by underlining the name (for italics) at its first mention (excluding headings) in the Experimental section only, and by giving analytical results in the form: (Found: C, 63.1; H, 5.4.  $C_{13}H_{13}NO_4$  requires C, 63.2; H, 5.3%). If analytical results for compounds which have been adequately described in the literature are to be included, they should be given in the form: (Found: C, 62.95; H, 5.4. Calc. for  $C_{13}H_{13}NO_4$ : C, 63.2; H, 5.3%). Analyses are normally quoted to the nearest 0.1%, but a '5' in the second place of decimals is retained.

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].

**U.v. absorptions.** These are given in the form  $\lambda_{max}$  (EtOH) 228 ( $\epsilon$  40 900 dm<sup>3</sup> mol<sup>-1</sup> cm<sup>-1</sup>), 262 (19 200), and 302 nm (11 500). Inflections and shoulders are specified as 228infl or 262sh. Alternatively the following form may be used:  $\lambda_{max}$  (EtOH) 228, 262, and 302 nm ( $\epsilon$  40 900, 19 200, and 11 500 dm<sup>3</sup> mol<sup>-1</sup> cm<sup>-1</sup>). Log  $\epsilon$  may be quoted instead of  $\epsilon$ .

**I.r. absorptions.** Shown as follows:  $\nu_{max}$  3 460 and 3 330 (NH), 2 200 (conj. CN), 1 650 (CO), and 1 620 cm<sup>-1</sup> (C=N). The type of signal (s, w, vs, br) can be indicated by appended letters (e.g. 1 760vs).

**N.m.r. data.** For all spectra  $\delta$  values should be used, with the nucleus indicated by subscript if necessary (e.g.  $\delta_H$ ,  $\delta_C$ ). Instrument frequency, solvent, and standard should be specified. For example:  $\delta_H$  (100 MHz; solvent CDCl<sub>3</sub>; standard Me<sub>4</sub>Si) 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 Hz,  $J_{AB}$  4 Hz, (iv) assignment; underlining for italics can be used to specify the nuclei concerned (e.g. CH<sub>3</sub>CH<sub>2</sub>). 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  $\rightarrow$  174), 147(176  $\rightarrow$  161), etc. The type of spectrum (field desorption, electron impact, etc.) should be indicated.

**Literature citations.** If comparison is to be made with literature values, these should be quoted in parentheses, e.g. m.p. 157 °C (from chloroform) (lit.,<sup>19</sup> 156 °C), or  $\nu_{max}$  2 020 and 1 592 cm<sup>-1</sup> (lit.,<sup>24</sup> 2 015 and 1 600 cm<sup>-1</sup>).

**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 ml) was oxidised with Jones' reagent (16 mmol) at room temperature for 4 h.

Table 0. Analytical data for the thioamides (28)—(36)

Compound (Formula)	Yield (%)	Solvent	M.p. (°C) (decomp.)	Found (%) (Required)		
				C	H	N
(28) (C <sub>22</sub> H <sub>16</sub> INO <sub>5</sub> S <sub>3</sub> )	69	MeOH	168—169	44.1 (44.2)	2.75 2.7	2.3 (2.3)
(29) (C <sub>22</sub> H <sub>16</sub> CINO <sub>5</sub> S <sub>3</sub> )	65	MeOH	168—170	52.4 (52.2)	3.0 3.2	2.7 (2.8)
(30) (C <sub>23</sub> H <sub>18</sub> INO <sub>2</sub> S <sub>3</sub> )	63	aq. Me <sub>2</sub> CO	162—163	45.35 (45.2)	2.9 2.0	2.3 (2.3)
(31) (C <sub>22</sub> H <sub>15</sub> CINO <sub>5</sub> S <sub>3</sub> )	70	MeOH	164—165	41.8 (41.8)	2.4 2.4	2.2 (2.2)
(32) (C <sub>24</sub> H <sub>20</sub> INO <sub>5</sub> S <sub>3</sub> )	67	MeOH	139—140	46.3 (46.1)	3.05 3.2	2.15 (2.2)
(33) (C <sub>25</sub> H <sub>22</sub> INO <sub>5</sub> S <sub>3</sub> )	57	EtOH	102—103	47.1 (46.95)	3.35 3.5	2.1 (2.2)
(34) (C <sub>33</sub> H <sub>22</sub> INO <sub>3</sub> S <sub>3</sub> )	41	AcOEt	174—175	56.6 (56.3)	3.0 3.15	1.8 (2.0)
(35) (C <sub>22</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>5</sub> S <sub>3</sub> )	43	EtOH	170—171	48.9 (48.9)	2.5 2.8	2.5 (2.6)
(36) (C <sub>19</sub> H <sub>18</sub> CINO <sub>5</sub> S <sub>3</sub> )	58	MeOH	159—150	48.1 (48.35)	3.9 3.8	3.0 (3.0)

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 (b.p. 40–60 °C) (1:1) as eluant yielded *vulgarin* (**21**) (11 mg, 27%), m.p. 176–177 °C (Found: C, 68.35; H, 7.75. C<sub>15</sub>H<sub>20</sub>O<sub>4</sub> requires C, 68.15; H, 7.5%);  $[\alpha]_D^{25} + 39^\circ$  (*c* 0.3 in CHCl<sub>3</sub>);  $\nu_{\max}$ . (CHCl<sub>3</sub>) 3 520 (OH), 1 780 ( $\gamma$ -lactone), and 1 675 cm<sup>-1</sup> ( $\alpha,\beta$ -unsaturated ketone);  $\lambda_{\max}$ . (EtOH) 215 nm;  $\delta_H$  (90 MHz; CDCl<sub>3</sub>) 1.23 (3 H, s, 10-Me), 1.28 (3 H, d, *J* 7 Hz, 11-Me), 1.55 (3 H, s, 4-Me), 2.36 (1 H, d, *J* 10 Hz, 5-H), 4.25 (1 H, dd, *J* 9 and 10 Hz, 6-H), 5.90 (1 H, d, *J* 10 Hz, 2-H), and 6.62 (1 H, d, *J* 10 Hz, 3-H); *m/z* 264 (*M*<sup>+</sup>, 100%) and 246 (*M*<sup>+</sup> - 18).

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

### 3.6 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 characterised, (*d*) if, earlier, it has been assigned an erroneous constitution, or (*e*) if it is a natural product isolated or synthesised for the first time. In preliminary communications compounds are often recorded with limited characterising 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 compounds, 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.

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

The position of the superior numerical 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,<sup>3</sup> 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<sup>3</sup> . . . should be written as ' . . . which gave a value<sup>3</sup> of 2.3 cm<sup>3</sup> ' or ' . . . which gave a value of 2.3 cm (ref. 3) '.

Since it is difficult to predict the final position of a table in the text, references cited only in the table should be incorporated into the printed footnotes to the table. References which are also cited elsewhere in the text should be referred to in the footnotes by the numbers used in the text citations, e.g. <sup>a</sup> Ref. 15.

*Journals.* The style of journal abbreviations to be used in the Society's publications is that defined in Chemical Abstracts Service Source Index (CASSI). The abbreviations listed in CASSI are based upon internationally recognised systems. The list of CASSI-style abbreviations on pages xii–xiii covers most 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 2 000 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 quotation marks, in upright letters, 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: B.P. 367 450, 367 455–7, U.S.P. 1 171 230. G.P. 436 112–4, Jap. P. 20 101. Dates are indicated thus: B.P. 666 776/1956. Patents which are applied for must always be given a year, e.g. B.P. Appl. 102/1982.

*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 (2/556).

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.*

## Journal Abbreviations

Acc. Chem. Res.  
Acta Acad. Abo, Ser. B  
Acta Biochim. Biophys. Acad. Sci. Hung.  
Acta Biochim. Iran.  
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 Metall.  
Acta Phys. Acad. Sci. Hung.  
Acta Phys. Chem.  
Acta Vitaminol. Enzymol.  
Adv. Act. Anal.  
Adv. Alicyclic Chem.  
Adv. Anal. Chem. Instrumen.  
Adv. Carbohydr. Chem. Biochem.  
Adv. Catal.  
Adv. Chem. Phys.  
Adv. Chromatogr.  
Adv. Colloid Interface Sci.  
Adv. Enzymol. Relat. Areas Mol. Biol.  
Adv. Free-Radical Chem.  
Adv. Heterocycl. Chem.  
Adv. Inorg. Bioinorg. Mech.  
Adv. Inorg. Chem. Radiochem.  
Adv. Lipid Res.  
Adv. Macromol. Chem.  
Adv. Magn. Reson.  
Adv. Molten Salt Chem.  
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.  
Agrokem. Talajtan  
AlChE J.  
Ambix  
Am. J. Pharm.  
Am. J. Sci.  
An. Acad. Bras. Cienc.  
Anal. Biochem.  
Anal. Chem.  
Anal. Chim. Acta  
Anal. Lett.  
Analysis  
Analyst (London)  
An. Bromatol.  
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  
Ann. Univ. Mariae Curie-Sklodowska, Sect. A  
AA  
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.  
Arzheim.-Forsch.  
Aspects Homogeneous Catal.  
At. Absorb. Newsl.  
Aust. J. Biol. Sci.  
Aust. J. Chem.  
Aust. J. Phys.  
Azerb. Khim. Zh.  
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.  
Bochu-Kagaku  
Boll. Soc. Ital. Biol. Sper.  
Br. Corros. J.  
Br. J. Pharmacol.  
Br. Polym. J.  
Bull. Inst. Politeh. Iasi.  
Bull. Acad. Sci. USSR, Div. Chem. Sci.  
Bull. Chem. Soc. Jpn.  
Bull. Inst. Chem. Res., Kyoto Univ.  
Bull. Pol. Acad. Sci., Chem.  
Bull. Sci., Cons. Acad. Sci. Arts RSF Yougosl., Sect. A  
Bull. Soc. Chim. Belg.  
Bull. Soc. Chim. Fr.  
Bunseki Kagaku  
Can. Chem. News  
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.  
Cereal Chem.  
Cesk. Farm.  
Chelates Anal. Chem.  
Chem. Age (London)  
Chem. Anal. (Warsaw)  
Chem. Ber.  
Chem. Br.  
Chem. Chron.  
Chem. Econ. Eng. Rev.  
Chem. Eng. Commun.  
Chem. Eng. J. (Lausanne)  
Chem. Eng. News  
Chem. Eng. Progr.  
Chem. Eng. (Rugby, Engl.)  
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. Listy  
Chem. Nat. Compd. (Engl. Transl.)  
Chem. N.Z.  
Chem. Pharm. Bull.  
Chem. Phys.  
Chem. Phys. Carbon  
Chem. Phys. Lett.  
Chem. Phys. Lipids  
Chem. Prum.  
Chem. Rev.  
ChemSA  
Chem. Scr.  
Chem. Soc. Rev.  
Chem. Siosow.  
Chem. Tech. (Leipzig)  
Chem. Technol.  
Chem. Week.  
Chem. Weekbl.  
Chem.-Ztg.  
Chem. Zvesti  
Chim. Acta Turc.  
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.  
Combust. Flame  
Commun. Fac. Sci. Univ. Ankara  
Commun. R. Soc. Edinburgh, Phys. Sci.  
Comput. Chem.  
Coord. Chem. Rev.  
Corros. Sci.  
Cosmet. Perfum.  
CRC Crit. Rev. Biochem.  
C.R. Seances Acad. Sci.  
Crit. Rev. Anal. Chem.  
Croat. Chem. Acta  
C.R. Seances Soc. Biol. Ses Fil.  
Curr. Sci.  
DEFAZET-Dtsch. Farben-Z.  
Denki Kagaku yobi Kogyo Butsuri Kagaku  
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  
Double-Liaison  
Dtsch. Lebensm.-Rundsch.  
Dyn. Mass Spectrom.  
Educ. Chem.  
Egypt. J. Chem.  
Electroanal. Chem.  
Electrochim. Acta  
Elektrokimiya  
Endeavour  
Environ. Sci. Technol.  
Erdol. Kohle, Erdgas, Petrochem., Brennst. Chem.  
Essays Biochem.  
Eur. J. Biochem.  
Eur. Polym. J.  
Experientia  
Faraday Discuss. Chem. Soc.  
Faraday Symp. Chem. Soc.

FEBS Lett.  
Fermentn. Spirt. Prom.  
Fette, Seifen, Anstrichm.  
Chem. Listy  
Finn Chem. Lett.  
Fiz.-Khim. Mekh. Mater.  
Fiz. Met. Metalloved.  
Flavour Ind.  
Fluorine Chem. Rev.  
Food Manuf.  
Fortsschr. Chem. Org. Naturst.  
Fortsschr. Hochpolym.-Forsch.  
Fresenius' Z. Anal. Chem.  
Fuel  
Gazz. Chim. Ital.  
Gen. Cytochem. Methods  
Geokhimiya  
Ger. Chem. Eng. (Engl. Transl.)  
Gidrokhim. Mat.  
Glas. Hem. Drus., Beograd  
Glass Technol.  
G. Microbiol.  
God. Viss. Khim.-Tekhnol. Inst., Sofia  
Grasas Aceites (Seville)  
Helv. Chim. Acta  
Heterocycles  
High Energy Chem. (Engl. Transl.)  
Hist. Stud. Phys. Sci.  
Hoppe-Seyler's Z. Physiol. Chem.  
Hua Hsueh  
Huaxue Tongbao  
Huaxue Xuebao  
Hung. J. Ind. Chem.  
Hwahak Kwa Kongop Ui Chinbo  
Ind. Eng. Chem., Fundam.  
Ind. Eng. Chem., Process. Des. Dev.  
Ind. Eng. Chem., Prod. Res. Dev.  
Indian J. Agric. Chem.  
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. Flavours Food Addit.  
Int. J. Appl. Radiat. Isot.  
Int. J. Chem. Kinet.  
Int. J. Mass Spectrom. 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.  
Istanbul Univ. Fen Fak. Mecm., Seri C  
Ital. J. Biochem.  
Itsuu Kenkyusho Nempo  
Izv. Akad. Nauk Kaz. SSR, Ser. Khim.  
Izv. Akad. Nauk SSSR, Neorg. Mater.  
Izv. Akad. Nauk SSSR, Ser. Khim.  
Izv. Akad. Nauk Turk. SSR, Ser. Fiz.-Tekh., Khim. Geol. Nauk  
Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk  
J. Agric. Food Chem.  
J. Am. Chem. Soc.



Journal Abbreviations (*continued*)

- J. Am. Leather Chem. Assoc.*  
*J. Am. Oil 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. Off. Anal. Chem.*  
*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. 1*  
*J. Chem. Soc., Faraday Trans. 2*  
*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. Coord. Chem.*  
*J. Cryst. Mol. Struct.*  
*J. Doc.*  
*J. Electroanal. Chem. Interfacial Electrochem.*  
*J. Electrochem. Soc.*  
*J. Electrochem. Soc. India*  
*J. Fac. Sci. Univ. Tokyo*  
*J. Fluorine Chem.*  
*J. Food Sci.*  
*J. Franklin Inst.*  
*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. Brew.*  
*J. Inst. Chem. (India)*  
*J. Inst. Fuel*  
*J. Labelled Compd. Radiopharm.*  
*J. Less-Common Met.*  
*J. Lipid Res.*  
*J. Liq. Chromatogr.*  
*J. Lumin.*  
*J. Macromol. Sci., Chem.*  
*J. Macromol. Sci., Phys.*  
*J. Magn. Reson.*  
*J. Med. Chem.*  
*J. Mol. Biol.*  
*J. Mol. Catal.*  
*J. Mol. Spectrosc.*  
*J. Mol. Struct.*  
*J. Neurochem.*  
*J. Nonmet. Semiconduct.*  
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*J. Polym. Sci., Polym. Symp.*  
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*J. Protein Chem.*  
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*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. Dyers Colour.*  
*J. Soc. Leather Technol. Chem.*  
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*J. Struct. Chem. (Engl. Transl.)*  
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*Kagaku Kagaku*  
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*Khim. Ind. (Sofia)*  
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*Nature (London)*  
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*Xenobiotica*  
  
*Yakugaku Zasshi*  
*Yuki Gosei Kagaku Kyokaiishi*  
  
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*Zavod. Lab.*  
*Zb. Pr. Chemickotechnol. Fac. SVST*  
*Z. Chem.*  
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*Zh. Anal. Khim.*  
*Zh. Eksp. Teor. Fiz.*  
*Zh. Eool. Biokhim. Fiziol.*  
*Zh. Fiz. Khim.*  
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*Zh. Neorg. Khim.*  
*Zh. Obshch. Khim.*  
*Zh. Org. Khim.*  
*Zh. Prikl. Khim. (Leningrad)*  
*Zh. Prikl. Spektrosk.*  
*Zh. Strukt. Khim.*  
*Zh. Vses. Khim. Ova im D.I. Mendeleeva*  
*Z. Kristallogr.*  
*Z. Lebensm.-Unters. Forsch.*  
*Z. Naturforsch., A*  
*Z. Naturforsch., B*  
*Z. Naturforsch., C*  
*Z. Phys. Chem. (Munich)*  
*Z. Phys. Chem. (Leipzig)*  
*Z. Vitam., Horm., Fermentforsch.*  
*Z. Wiss. Photogr., Photophys., Photochem.*

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, *ibid.*, 1957, 79, 567; A. B. Jones and E. F. Green, *ibid.*, p. 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 <sup>1,2</sup>); 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.

(Note: *ibid.* is used only within a given reference and not to refer from one reference number to another: the abbreviated title for the journal should be repeated for separate reference numbers.)

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

### 3.8 Nomenclature

For many years the Society has actively encouraged the use of standard IUPAC nomenclature and symbolism in its publication 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

**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

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.

Nomenclature of Inorganic Chemistry, Butterworths, London, 1971 (now published by Pergamon).

Biochemical Nomenclature and Related Documents, The Biochemical Society, London, 1978.

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.

### 3.9 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, 1988 edn.).

**Guidelines for the publications of the Society.** An author will not be denied any reasonable usage, but 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.

**Table 2.** Prefixes

Fraction	Prefix	Symbol	Multiple	Prefix	Symbol
10 <sup>-1</sup>	deci	d	10	deka	da
10 <sup>-2</sup>	centi	c	10 <sup>2</sup>	hecto	h
10 <sup>-3</sup>	milli	m	10 <sup>3</sup>	kilo	k
10 <sup>-6</sup>	micro	μ	10 <sup>6</sup>	mega	M
10 <sup>-9</sup>	nano	n	10 <sup>9</sup>	giga	G
10 <sup>-12</sup>	pico	p	10 <sup>12</sup>	tera	T
10 <sup>-15</sup>	femto	f			
10 <sup>-18</sup>	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	kg m <sup>2</sup> s <sup>-2</sup>
force	newton	N	kg m s <sup>-2</sup> = J m <sup>-1</sup>
power	watt	W	kg m <sup>2</sup> s <sup>-3</sup> = J s <sup>-1</sup>
electric charge	coulomb	C	A s
electric potential			
difference	volt	V	kg m <sup>2</sup> s <sup>-3</sup> A <sup>-1</sup> = J A <sup>-1</sup> s <sup>-1</sup>
electric resistance	ohm	Ω	kg m <sup>2</sup> s <sup>-3</sup> A <sup>-2</sup> = V A <sup>-1</sup>
electric capacitance	farad	F	A <sup>2</sup> s <sup>4</sup> kg <sup>-1</sup> m <sup>-2</sup> = A s V <sup>-1</sup>
magnetic flux	weber	Wb	kg m <sup>2</sup> s <sup>-2</sup> A <sup>-1</sup> = V s
inductance	henry	H	kg m <sup>2</sup> s <sup>-2</sup> A <sup>-2</sup> = V A <sup>-1</sup> s
magnetic flux density	tesla	T	kg s <sup>-2</sup> A <sup>-1</sup> = V s m <sup>-1</sup>
luminous flux	lumen	lm	cd sr
illumination	lux	lx	cd sr m <sup>-2</sup>
frequency	hertz	Hz	s <sup>-1</sup>

**Table 4.** Derived units with no special names or symbols

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

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 m.k.s.) units. If authors wish to use equations suitable for e.s.u. or e.m.u. the lack of consistency with SI units must be explicitly noted.

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

(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, p. xiv). 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 (p. xiv). 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.

**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 <sup>-10</sup> m = 10 <sup>-1</sup> nm
length	micron	μm	10 <sup>-6</sup> m
area	barn	b	10 <sup>-28</sup> m <sup>2</sup>
volume	litre	l	10 <sup>-3</sup> m <sup>3</sup> = dm <sup>3</sup>
mass	tonne	t	10 <sup>3</sup> kg = Mg
force	dyne	dyn	10 <sup>-5</sup> N
pressure	bar	bar	10 <sup>5</sup> N m <sup>-2</sup>
pressure	pascal	Pa	N m <sup>-2</sup>
energy	erg	erg	10 <sup>-7</sup> J
kinematic viscosity, diffusion coefficient	stokes	St	10 <sup>-4</sup> m <sup>2</sup> s <sup>-1</sup>
dynamic viscosity	poise	P	10 <sup>-1</sup> kg m <sup>-1</sup> s <sup>-1</sup>
magnetic flux	maxwell	Mx	10 <sup>-8</sup> Wb
magnetic flux density (magnetic induction)	gauss	G	10 <sup>-4</sup> T
conductance	siemens	S	Ω <sup>-1</sup>

(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 to SI units are subject to change in the light of new experimental measurements of the constants involved. Their use outside the restricted 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	eV = 1.6021 × 10 <sup>-19</sup> J
mass	unified atomic mass unit	u	u = 1.660 41 × 10 <sup>-27</sup> 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 (see p. xvi) is by no means exhaustive. Each of the definitions given in the fourth column is *exact*.

### 3.10 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 on p. xvi):

(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.

**Table 6.** Units defined in terms of SI units

Physical quantity	Name of unit	Symbol for unit	Definition of unit
length	inch	in	$2.54 \times 10^{-2}$ m
mass	pound (avoirdupois)	lb	0.453 592 37 kg
time*	minute	min	60 s
time*	hour	h	3 600 s
force	kilogram-force	kgf	9.806 65 N
force	pound-force	lbf	$9.806 65 \times 0.453 592 37$ N
pressure	atmosphere	atm	$101 325$ N m <sup>2</sup>
pressure	conventional millimetre of mercury	mmHg	$13.5951 \times 9.806 65$ N m <sup>-2</sup>
pressure	torr	Torr	$(101 325/760)$ N m <sup>-2</sup>
pressure	pound-force per square inch	lbf in <sup>-2</sup>	$\frac{9.806 65 + 4 535.9237}{6.4516}$ N m <sup>-2</sup>
energy	kilowatt hour	kW h	$3.6 \times 10^4$ J
energy	thermochemical calorie	cal(thermochem.)	4.184 J
energy	I.T. calorie	cal <sub>IT</sub>	4.1868 J
thermodynamic temperature	degree Rankine	°R	(5/9) K
radioactivity	curie	Ci	$3.7 \times 10^{16}$ s <sup>-1</sup>

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

### Specimen first page of typescript

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Inclusion Properties of Structures of the Type (RSC)<sub>n</sub>

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The clathrating ability of various structures of the type (RSC)<sub>n</sub> has been studied. Hexakis(alkylthio)benzenes, (RSC)<sub>6</sub>, exhibit considerable activity as host molecules, and exceptional stability is conferred by SAC substituents

Recent reports of inclusion behaviour by hexakis(phenylthio)-benzene, (PhSC)<sub>6</sub>,<sup>1</sup> and some initial studies by R.S. Cahn,<sup>2</sup> led us to investigate the host-guest chemistry of further structures of the type (RSC)<sub>n</sub>. We were particularly interested in the benzene derivatives (RSC)<sub>6</sub>, which were expected to possess an attractive divisional structure.

The multi-step synthesis of (RSC)<sub>6</sub>, carried out over a period of several years, was achieved.....

## (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 3.3.6.

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

#### 4.0 Deposition of Data: Supplementary Publications Scheme

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 U.K. and abroad on quoting a supplementary publication number that will appear in the parent article.

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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.

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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.

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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.

#### 5.0 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.

##### 5.1 Title and Summary

The title of a paper reporting a crystallographic structure determination should normally contain the words 'Crystal Structure of...'

The summary need not contain cell dimensions and other crystal data, but should make clear that a crystal structure analysis has been performed.

##### 5.2 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 ( $\mu$ ).

##### 5.3 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.

## 5.4 Structure Analysis and Refinement

The information provided should fulfil the same criteria as for data collection (section 5.3). 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.

## 5.5 Example of Presentation

The following example demonstrates the application of the recommendations in the preceding sections (5.2 to 5.4):

### Experimental

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

*Crystal Data.*— $C_{24}H_{26}Cl_3Re_3Si_6$ ,  $M = 1028.0$ . Monoclinic,  $a = 12.021(3)$ ,  $b = 20.489(5)$ ,  $c = 18.194(5)$  Å,  $\beta = 91.03(3)^\circ$ ,  $V = 4480$  Å<sup>3</sup> (by least-squares refinement on diffractometer angles for 15 automatically centred reflections,  $\lambda = 0.71069$  Å), space group  $P2_1/n$  (alt.  $P2_1/c$ , No. 14),  $Z = 4$ ,  $D_x = 1.76$  g cm<sup>-3</sup>. Dark blue, air-sensitive tablets. Crystal dimensions (distance to faces from centre):  $0.313(211, \bar{2}\bar{1}\bar{1}) \times 0.163(010, \bar{0}\bar{1}\bar{0}) \times 0.063(101, \bar{1}\bar{0}\bar{1})$  mm,  $\mu(Mo-K\alpha) = 85.12$  cm<sup>-1</sup>.

*Data Collection and Processing.*<sup>12</sup>—CAD4 diffractometer,  $\omega/2\theta$  mode with  $\omega$  scan width =  $0.85 + 0.35 \tan \theta$ ,  $\omega$  scan speed 1.3–6.8 deg min<sup>-1</sup>, graphite-monochromated Mo- $K\alpha$  radiation; 6383 reflections measured ( $1.5 \leq \theta \leq 25^\circ$ ,  $+h,k,l$ ), 5797 unique [merging  $R = 0.024$  after absorption correction (max., min. transmission factors = 0.37, 0.10)], giving 4170 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  $\mu_{iso}$  [=  $0.08(2)$  Å<sup>2</sup>]. The weighting scheme  $w = 1/[\sigma^2(F_o) + 0.0078F_o^2]$ , with  $\sigma(F_o)$  from counting statistics<sup>12</sup> 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.

## 5.6 Presentation of Tables and Diagrams

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

5.6.1 *For Publication in the Journal.*—(1) A table of final fractional atomic co-ordinates (labelled  $x, y, z$ ) must be included. If the origin chosen differs from that adopted in International Tables this should be mentioned and justified. Where the asymmetric unit consists of a discrete molecule (or molecules) co-ordinates should refer to atoms which are all in the same molecule. Hydrogen atom co-ordinates should be included only when experimentally determined or refined; when they have been determined only by calculation, deposition is appropriate.

(2) A table of selected bond lengths and angles, with estimated standard deviations. This should be restricted to significant dimensions only (for example it is rarely necessary to include data for phenyl rings). Average values may be given (with a range of e.s.d.s) for chemically equivalent groups or for similar bonds. As an alternative to tabular presentation it is often clearer to give important dimensions in a structural diagram. Differences from expected norms should be noted.

(3) 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<sup>I</sup>) ••• C(2<sup>IV</sup>).

5.6.2 *For the Referees and/or for Deposition.*—(1) Any calculated co-ordinates (e.g. hydrogen).

(2) A full list of bond lengths and angles with estimated standard deviations.

(3) A full list of thermal parameters in the form  $B_{ij}$  or  $U_{ij}$  (in Å<sup>2</sup> or pm<sup>2</sup>).

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

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

5.6.3 *Deposition of Material at the Cambridge Crystallographic Data Centre.*—The table of final fractional atomic co-ordinates, the full list of bond lengths and angles, and the list of thermal parameters will be deposited at the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW (or at the Institut für Anorganische Chemie, Universität, Gerhard-Domagk-Str. 1, D-5300 Bonn, via Prof. Dr. G. Bergerhoff, for molecules not containing 'organic' carbon). All Tables should be of publication quality. Computer printout is acceptable provided that it is clearly legible. The print program used should yield

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

concise tables of atomic and other derived parameters. The content of the tables should be non-redundant, and their interpretation immediately obvious. The thermal parameters should be submitted as separate tables, with clear definition of the units used. Any request to Cambridge or to Bonn for deposited material should be accompanied by the full literature citation for the paper concerned.

### 5.7 Reference to Crystallographic Work Published in *Chemical Communications*

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

### 5.8 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 co-ordinates *etc.* will be deposited at the Cambridge Crystallographic Data Centre (or Bonn). The brief published description of the determination should be supplemented by appropriate reference to 'unpublished work'.

### 6.0 Perkin Communications

Preliminary accounts of novel and significant work of exceptional interest may be published in *Perkin Transactions 1* 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, should 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 2 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.

Times to publication will be similar to those for *Chemical Communications*. In order to achieve this, failure of an author to produce a revised script in response to referees' comments within 4 weeks will be regarded as a withdrawal of the Communication. Furthermore, proof corrections received more than 2 weeks after despatch of proofs by the printer will not be incorporated.

### 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 II*, one in which the computations are incidental to the chemistry to *Perkin, Dalton*, or *Faraday Transactions I*. 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 semi-empirical 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 he considers the method adequate for 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.