JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANSACTIONS

Instructions for Authors (1983)

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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*). Radiation chemistry, gas-phase kinetics, electrochemistry (other than preparative), surface and interfacial chemistry, heterogeneous catalysis, physical properties of polymers and their solutions, and kinetics of polymerisation, *etc.*

Faraday Transactions II (*Chemical Physics*). Theoretical chemistry, especially valence and quantum theory, statistical mechanics, intermolecular forces, relaxation phenomena, spectroscopic studies (including i.r., e.s.r., n.m.r., and kinetic spectroscopy, *etc.*) leading to assignments of quantum states, and fundamental theory. Studies of impurities in solid systems.

Perkin Transactions I (*Organic Chemistry*). All aspects of synthetic and natural product organic, organometallic, and bio-organic chemistry, including aliphatic, alicyclic, and aromatic systems (carbocyclic and heterocyclic).

Perkin Transactions II (*Physical Organic Chemistry*). Kinetic and mechanistic studies of organic, organometallic, and bio-organic reactions. The description and application of physicochemical, spectroscopic, and theoretical procedures to organic chemistry, including structure–activity relationships. Physical aspects of bio-organic chemistry and of organic compounds, including polymers and biopolymers.

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.

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.*

1.2 Submission of Articles

Typescripts should be addressed to: The Manager, Journals, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN.

Three copies of the typescript (a top copy and two good quality carbon or Xerox copies) are required.

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.

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, 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.[1] Preparation and Reactions of Pyrazine *N*-Oxides.

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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.

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. 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^{-3}; 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, β-chlorophenethylbenzene, tri-μ-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*-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 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, Discussions, *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 by 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.

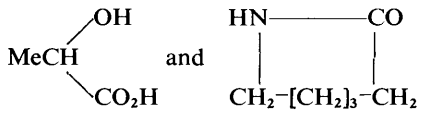
(*b*) Formulae should be numbered with arabic numerals in parentheses [(1), (2), and (3) *etc.*] in the order in which they are displayed and not in the order of mention in text.

(*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.*

$HO{-}CHMe{-}CO_2H$ and $\overline{NH{-}[CH_2]_5{-}CO}$ 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*-$HO{-}C_6H_4{-}CH_2{-}NH_2$ and $CH_2Cl{-}CH(OH){-}CO_2H$.

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.

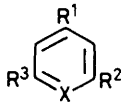
Repeating sequences of a backbone composite group are enclosed in square brackets and their number is indicated by an inferior multiplier, *e.g.* $HO[CH_2]_4NH_2$, but $HO[CH_2]_4N(CH_2OH)_2$.

(*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 – – – – or ||||.

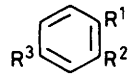
(*h*) The abbreviations Me, Et, Pr^n, Pr^i, Bu^n, Bu^i, Bu^s, Bu^t, Ph, Ac, Alk, Ar, and Hal, should be used except when the group is involved in the reaction described. Other special symbols, if used, require an explanatory footnote. The carboxy-group is written CO_2H (not COOH); similarly CO_2R.

(*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) $R^1 = R^2 = Ph$, $R^3 = Me$, X = O
(2) $R^1 = Me$, $R^2 = R^3 = Ph$, X = S



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

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 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.* $\ln(p/\text{atm})$, $10^3(T/K)^{-1}$.

(*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, their presentation in tabular form is preferred. No standard rules for the economical layout of tables can be provided, but authors will find it helpful to consult recent issues of the *Journal* for examples.

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.* $\ln(p^m/\text{atm})$,

Example:

θ/°C	T/K	$10^3\text{K}/T$	p/atm	$\ln(p/\text{atm})$	$V_m^G/\text{cm}^3\ \text{mol}^{-1}$	pV_m^G/RT
−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.* $\dfrac{V_m^G}{\text{cm}^3\ \text{mol}^{-1}}$ 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° (*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 0.05%.

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 (ε 40 900 dm^3 mol^{-1} cm^{-1}), 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 (ε 40 900, 19 200, and 11 500 dm^3 mol^{-1} cm^{-1}). Log ε may be quoted instead of ε.

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^{-1} (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 δ values should be used, with the nucleus indicated by subscript if necessary (*e.g.* δ_H, δ_C). Instrument frequency, solvent, and standard should be specified. For example: δ_H (100 MHz; solvent $CDCl_3$; standard 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 Hz, J_{AB} 4 Hz, (iv) assignment; underlining for italics can be used to specify the nuclei concerned (*e.g.* CH_3CH_2). The proton attached to C-6 may be designated C(6)H or 6-H; the methyl attached to C-6, 6-Me or C(6)Me.

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 ⟶ 174), 147 (176 ⟶ 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.,[19] 156 °C), or $\nu_{max.}$ 2 020 and 1 592 cm^{-1} (lit.,[24] 2 015 and 1 600 cm^{-1}).

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.

> *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. 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. $C_{15}H_{20}O_4$ requires C, 68.15; H, 7.5%); $[\alpha]_D$ +39° (*c* 0.3 in $CHCl_3$); $\nu_{max.}$ ($CHCl_3$) 3 520 (OH), 1 780 (γ-lactone), and 1 675 cm^{-1} (α,β-unsaturated ketone); $\lambda_{max.}$ (EtOH) 215 nm; δ_H (90 MHz; $CDCl_3$) 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^+, 100%) and 246 ($M^+ - 18$).

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

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

Compound (Formula)	Yield (%)	Solvent	M.p. (°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
($C_{23}H_{18}INO_5S_3$)				(45.2	2.0	2.3)
(31)	70	MeOH	164—165	41.8	2.4	2.2
($C_{22}H_{15}ClNO_5S_3$)				(41.8	2.4	2.2)
(32)	67	MeOH	139—140	46.3	3.05	2.15
($C_{24}H_{20}INO_5S_3$)				(46.1	3.2	2.2)
(33)	57	EtOH	102—103	47.1	3.35	2.1
($C_{25}H_{22}INO_5S_3$)				(46.95	3.5	2.2)
(34)	41	AcOEt	174—175	56.6	3.0	1.8
($C_{33}H_{22}INO_3S_3$)				(56.3	3.15	2.0)
(35)	43	EtOH	170—171	48.9	2.5	2.5
($C_{22}H_{15}Cl_2NO_5S_3$)				(48.9	2.8	2.6)
(36)	58	MeOH	159—150	48.1	3.9	3.0
($C_{19}H_{18}ClNO_5S_3$)				(48.35	3.8	3.0)

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 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 . . .'. It may be necessary to modify this rule, however, to avoid confusion, thus: ' In this way the method was found to be suitable for lead [2], tin [3], bismuth [4], and mercury [5].'

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) '.

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.* [a] 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 authoritiative 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 data.

Names. The names and initials of all authors are always given in the reference footnote; 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.

Journal Abbreviations

Acc. Chem. Res.
Acta Acad. Aboensis, 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.
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. 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
AIChE J.
Ambix
Am. J. Pharm.
Am. J. Sci.
An. Acad. Bras. Cienc.
Anal. Biochem.
Anal. Chem.
Anal. Chim. Acta
Anal. Lett.
Analusis
Analyst (London)
An. Bromatol.
Angew. Chem.
Angew. Chem., Int. Ed. Engl.
Angew. Makromol. Chem.
Ann. Acad. Sci. Fenn., Sect. AII, Chem.
Ann. Chim. (Paris)
Ann. Chim. (Rome)
Ann. Endocrinol.
Ann. N.Y. Acad. Sci.
Ann. Pharm. Fr.
Ann. Soc. Sci. Bruxelles
Ann. Univ. Mariae Curie-Sklodowska, Sect. AA
Annu. Rep. Anal. At. Spectrosc.
Annu. Rep. Med. Chem.
Annu. Rep. Prog. Chem., Sect. A, Phys. Inorg. Chem.
Annu. Rep. Prog. Chem., Sect. B.
Annu. Rev. Biochem.
Annu. Rev. Ind. Eng. Chem.
Annu. Rev. NMR Spectrosc.
Annu. Rev. Phys. Chem.
Appl. Spectrosc.
Arch. Pharm. Chemi, Sci. Ed.
Arch. Pharm. (Weinheim, Ger.
Arm. Khim. Zh.
Arzneim.-Forsch.
Aspects Homogeneous Catal.
At. Absorpt. 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 (Engl. 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.
Bol. Soc. Quim. Peru
Br. Corros. J.
Br. J. Pharmacol.
Br. Polym. J.
Br. Polym. J.
Bul. Inst. Politeh. Iasi.
Bull. Acad. Pol. Sci., Ser. Sci. Chim.
Bull. Acad. Sci. USSR, Div. Chem. Sci.
Bull. Chem. Soc. Jpn.
Bull. Inst. Chem. Res., Kyoto Univ.
Bull. Sci., Cons. Acad. Sci. Arts RSF Yougosl., Sect. A
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.
Cereal Chem.
Cesk. Farm.
Chelates Anal. Chem.
Chem. Age (London)
Chem. Anal. (Warsaw)
Chem. Ber.
Chem. Br.
Chem. Can.
Chem. Chron.
Chem. Econ. Eng. Rev.
Chem. Eng. Commun.
Chem. Eng. J. (Lausanne)
Chem. Eng. (London)
Chem. Eng. News
Chem. Eng. Progr.
Chem. Eng. Progr., Monogr. Ser.
Chem. Eng. Progr., Symp. Ser.
Chem. Eng. Sci.
Chem. Erde
Chem. Heterocycl. Compd. (Engl. Transl.)
Chem. Ind. (Deusseldorf)
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. Soc., Spec. Publ.
Chem. Stosow.
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.
Corrosion Sci.
Cosmet. Perfum.
CRC Crit. Rev. Biochem.
C.R. Hebd. 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 Oyobi 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.)
Dopo. Akad. Nauk Ukr. RSR, Ser. B
Double-Liaison
Dtsch. Lebensm. -Rundsch.
Dyn. Mass Spectrom.

Educ. Chem.
Egypt. J. Chem.
Electroanal. Chem.
Electrochim. Acta
Elektrokhimiya
Endeavour
Environ. Sci. Technol.
Erdoel 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.
Finn Chem. Lett.
Fiz. -Khim. Mekh. Mater.
Fiz. Met. Metalloved.
Flavour Ind.
Fluorine Chem. Rev.
Food Manuf.
Fortschr. Chem. Org. Naturst.
Fortschr. Hochpolym. -Forsch.
Freseniusz 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. Vissh. Khimikotekhnol. Inst., Sofia
Grasas Aceites (Seville)

Helv. Chim. Acta
High Energy Chem. (Engl. Transl.)
Hist. Stud. Phys. Sci.
Hoppe-Seyler's Z. Physiol. Chem.
Hua Hsueh
Hua Hsueh Hsueh Pao
Hua Hsueh Tung Pao
Hung. J. Ind. Chem.
Hwahak Kwa Kongop Ui Chinbo

Ind. Eng. Chem., Fundam.
Ind. Eng. Chem., Process. Res. 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. Nucl. Chem. Lett.
Inorg. Synth.
Int. Chem. Eng.
Int. Flavours Food Addit.
Int. J. Appl. Radiat. Isot.
Int. J. Chem. Kinet.
Int. J. Mass Spectrom. Ion Phys.
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.

Journal Abbreviations *(continued)*

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 Turkm. SSR, Ser. Fiz. Tekh., Khim. Geol. Nauk
Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk

J. Agric. Food Chem.
J. Am. Chem. Soc.
J. Am. Leather Chem. Assoc.
J. Am. Oil Chem. Soc.
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., Nucleosides, Nucleotides
J. Catal.
J. Chem. Educt.
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. Nucl. Chem.
J. Inst. Brewing, London
J. Inst. Chem., Calcutta
J. Inst. Fuel
J. Labelled Comp. 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.
J. Oil Colour Chem. Assoc.
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., Macromol. Rev.
J. Polym. Sci., Polym. Chem. Ed.
J. Polym. Sci., Polym. Phys. Ed.
J. Polym. Sci., Polym. Symp.
J. Prakt. Chem.
J. Quant. Spectrosc. Radiat. Transfer
J. Radioanal. 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. AII, Phys., Chem.
J. Sci. Ind. Res.
J. Soc. Dyers Colour.
J. Soc. Leather Technol. Chem.
J. Solid State Chem.
J. Solution Chem.
J. Steroid Biochem.
J. Struct. Chem. (Engl. Transl.)
J. Text. Inst.
J. Therm. Anal.
Justus Liebigs Ann. Chem.

Kagaku Kogaku
Kanazawa Daigaku Yakugakubu Kenkyu Nempo
Kem. -Kemi
Kem. Tidskr.
Khim. Geterotsikl. Soedin.
Khim. Ind. (Sofia)
Khim. Neft. Mashinostr.
Khim. Prir. Soedin.
Khim. Prom. (Moscow)
Khim. Volokna
Khim. Vys. Energ.
Kinet. Catal. (Engl. Transl.)
Kinet. Katal.
Kjemi
Kobunshi Kagaku
Kogyo Kagaku Zasshi
Kolloidn. Zh.
Koord. Khim.
Kristallografiya
Kunstst. -Plast. (Solothurn, Switz.)

Lab. Pract.
Latv. PSR Zinat. Vestis, Kim. Ser.
Lipids

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

Nahrung
Nature (London)
Naturwissenschaften
Neftekhimiya
Nippon Kagaku Kaishi
Nippon Nogei Kagaku Kaishi
Nouv. J. Chim.

Oesterr. Chem. -Ztg.
Online (Weston. Conn.)
Orbital
Org. Magn. Reson.
Org. Mass Spectrom.
Org. Prep. Proced. Int.
Org. React.
Org. React. (USSR)
Org. React. Mech.
Org. Synth.

Paint Manuf.
Pak. J. Sci.
Pak. J. Sci. Ind. Res.
Pak. J. Sci. Res.
Periodia Polytech., Chem. Eng.
Pestic. Sci.
Philos. Mag.
Philos. Trans. R. Soc. London, Ser. A
Phosphorus Sulfur
Photochem. Photobiol.
Phys. Chem. Glasses
Phys. Rev.
Phys. Rev. Lett.
Phys. Scr.
Phytochemistry
Pigm. Resin Technol.
Pis'ma Zh. Eksp. Teor. Fiz.
Plast. Polym.
Pol. J. Chem.
Polym. Age
Polymer
Polym. Sci. USSR (Engl. Transl.)
Postepy Biochem.
Prikl. Biokhim. Mikrobiol.
Priroda (Moscow)
Proc. Am. Soc. Brew. Chem.
Proc. Anal. Div. Chem. Soc.
Process Biochem.
Processing
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, Ser. 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.
Prog. Surf. Membr. Sci.
Prog. Surf. Sci.
Prog. Thin-Layer Chromatogr. Relat. Methods
Przem. Chem.
Pure Appl. Chem.
Pyrethrum Post

Quad. Ing. Chim. Ital.
Quim. Nova

Radiat. Phys. Chem.
Radiat. Res.
Radiochim. Acta
Radiokhimiya
React. Kinet. Catal. Lett.
Recent Dev. Chem. Nat. Carbon Compd.
Recent Prog. Horm. Res.
Recherches
Recl. Trav. Chim. Pays-Bas
Rend. Accad. Sci. Fis. Mat., Naples
Rep. Prog. Appl. Chem.
Residue Rev.
Rev. Anal. Chem.
Rev. Asoc. Bioquim. Argent.
Rev. Chim. (Bucharest)
Rev. Phys. Chem. Jpn.
Rev. Port. Quim.
Rev. Roum. Biochim.
Rev. Roum. Chim.
Rev. Sci. Instrum.
Rev. Soc. Quim. Mex.
Ric. Sci.
Rubber Chem. Technol.
Russ. Chem. Rev. (Engl. Transl.)
Russ. J. Inorg. Chem. (Engl. Transl.)
Russ. J. Phys. Chem. (Engl. Transl.)

S. Afr. J. Chem.
Sankyo Kenkyusho Nempo
Sb. Ved. Pr., Vys. Sk. Chemickotechnol., Pardubice
Sch. Sci. Rev.
Schweiz. Apoth. -Ztg.
Sci. Cult.
Science
Sci. Pap. Coll. Gen. Educ., Univ. Tokyo
Sci. Pap. Inst. Phys. Chem. Res. (Jpn.)
Sci. Rep. Res. Inst., Tohoku Univ.
Sci. Rep. Tohoku Univ., Ser. 1
Sci. Sinica
Sel. Annu. Rev. Anal. Sci.
Semicond. Insul
Sep. Purif. Methods
Sep. Sci. Technol.
Soap. Cosmet., Chem. Spec.
Sov. Electrochem. (Engl. Transl.)
Sov. J. Bioorg. Chem. (Engl. Transl.
Sov. J. Coord. Chem. (Engl. Transl.)
Sov. Phys. -Crystallogr. (Engl. Transl.
Sov. Radiochem. (Engl. Transl.)
Spectrochim. Acta, Part A
Spectrochim. Acta, Part B
Spectrosc. Lett.
Steroids
Steroids Lipids Res.
Struct. Bonding (Berlin)
Stud. Univ. Babes-Bolyai, Ser. Chem.
Sub-Cell. Biochem.
Surf. Colloid Sci.
Surf. Sci.
Synth. Commun.
Synthesis
Synth. Proced. Nucleic Acid Chem.
Synth. React. Inorg. Metal-Org. Chem.

Taehan Hwahak Hoechi
Talanta
Technol. Rep. Osaka Univ.
Teor. Eksp. Khim.
Teor. Osn. Khim. Tekhnol.
Tetrahedron
Tetrahedron Lett.
Text. Inst. Ind.
Text. Res. J.
Theor. Exp. Chem. (Engl. Transl.
Thermochim. Acta
Tin Its Uses
Tokyo Kogyo Shikensho Hokoku
Top. Curr. Chem.
Top. Stereochem.
Trans. Inst. Chem. Eng.
Trans. Inst. Met. Finish.
Transition Met. Chem.
Trans. J. Br. Ceram. Soc.
Trends Biochem. Sci.
Tr. Inst. Elektrokhim., Ural. Nauchn. Tsentr. Akad. Nauk SSSR

Ukr. Biokhim. Zh.
Ukr. Khim. Zh. (Russ. Ed.)
Usp. Khim.
UV Spectrom. Group Bull.
Uzb. Khim. Zh.

Vestn. Leningr. Univ., Fiz., Khim.
Vestn. Mosk. Univ., Khim.
Vestn. Slov. Kem. Drus.
Vestsi Akad. Navuk B, SSR. Ser. Khim Navuk
Veszpremi Vegyip, Egy. Kozl.
Vitam. Horm. (N.Y.)
Vopr. Med. Khim.
Vysokomol. Soedin., Ser. A
Vysokomol. Soedin., Ser. B

Xenobiotica

Yakugaku Zasshi
Yuki Gosei Kagaku Kyokai Sh

Z. Anorg. Allg. Chem.
Zavod. Lab.
Zb. Pr. Chemickotechnol. Fac. SVST
Z. Chem.
Zentralbl. Pharm., Pharmakother. Laboratoriumsdiagn.
Zh. Anal. Khim.
Zh. Eksp. Teor. Fiz.
Zh. Evol. Biokhim. Fiziol.
Zh. Fiz. Khim.
Zh. Nauchn. Prikl. Fotogr. Kinematogr.
Zh. Neorg. Khim.
Zh. Obshch. Khim.
Zh. Org. Khim.
Zh. Prikl. Khim.
Zh. Prikl. Spektrosk.
Zh. Strukt. Khim.
Zh. Vses. Khim. Ova.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.
Z. Lebensm. -Unters. Forsch.
Z. Naturforsch., Teil A
Z. Naturforsch., Teil B
Z. Naturforsch., Teil C
Z. Phys. Chem. (Frankfurt am Main)
Z. Phys. Chem. (Leipzig)
Z. Vitam., Horm., Fermentforsch.
Z. Wiss. Photogr., Photophys., Photochem.

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 [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.

(*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 publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Although the IUPAC rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general.

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.

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

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

A complete listing of all 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 Symbols Committee of The Royal Society, of which The Royal Society of Chemistry is a participating member, has produced a set of recommendations in a pamphlet 'Quantities, Units, and Symbols,' 1975 (copies of this pamphlet and further details can be obtained from the Manager, Journals, The Royal Society of Chemistry, Burlington House, Piccadilly, London, W1V 0BN). These recommendations are applied by The Royal Society of Chemistry in all its publications. Their basis is the 'Système International d'Unités' (SI).

A more detailed treatment of units and symbols with specific application to chemistry is given in the IUPAC Manual of Symbols and Terminology for Physicochemical Quantities and Units (Pergamon, Oxford, 1979).

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.

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.

(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.

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	deka	da
10^{-2}	centi	c	10^{2}	hecto	h
10^{-3}	milli	m	10^{3}	kilo	k
10^{-6}	micro	μ	10^{4}	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	$kg\ m^2\ s^{-2}$
force	newton	N	$kg\ m\ s^{-1} = J\ m^{-1}$
power	watt	W	$kg\ m^2\ s^{-3} = J\ s^{-1}$
electric charge	coulomb	C	A s
electric potential difference	volt	V	$kg\ m^2\ s^{-3}\ A^{-1} = J\ A^{-1}\ s^{-1}$
electric resistance	ohm	Ω	$kg\ m^2\ s^{-3}\ A^{-2} = V\ A^{-1}$
electric capacitance	farad	F	$A^2\ s^4\ kg^{-1}\ m^{-2} = A\ s\ V^{-1}$
magnetic flux	weber	Wb	$kg\ m^2\ s^{-2}\ A^{-1} = V\ s$
inductance	henry	H	$kg\ m^2\ s^{-2}\ A^{-2} = V\ A^{-1}\ s$
magnetic flux density	tesla	T	$kg\ s^{-2}\ A^{-1} = V\ s\ m^{-2}$
luminous flux	lumen	lm	cd sr
illumination	lux	lx	$cd\ sr\ m^{-2}$
frequency	hertz	Hz	s^{-1}

Table 4. Derived units with no special names or symbols

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

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.

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}

(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	$eV = 1.6021 \times 10^{-19}\ J$
mass	unified atomic mass unit	u	$u = 1.660\,41 \times 10^{-27}\ kg$

(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 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.

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	3 600 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	I.T. calorie	cal_{IT}	4.1868 J
thermodynamic temperature	degree Rankine	°R	(5/9) K
radioactivity	curie	Ci	3.7×10^{16} s^{-1}

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

Specimen first page of typescript

Proofs to: W.H. Perkin
Royal Society of Chemistry,
Burlington House,
Piccadilly,
LONDON
W1V 0BN

Inclusion Properties of Structures of the Type $(RSC)_n$

John Dalton, Michael Faraday, and William H. Perkin *
Royal Society of Chemistry, Burlington House, Piccadilly,
London, W1V 0BN

The clathrating ability of various structures of the type $(RSC)_n$ has been studied. Hexakis(alkylthio)benzenes, $(RSC)_6$, exhibit considerable activity as host molecules, and exceptional stability is conferred by SAc substituents

Recent reports of inclusion behaviour by hexakis(phenylthio)-benzene, $(PhSC)_6$,[1] and some initial studies by R.S. Cahn,[2] led us to investigate the host-guest chemistry of further structures of the type $(RSC)_n$. We were particularly interested in the benzene derivatives $(RSC)_6$, which were expected to possess an attractive divisional structure.

The multi-step synthesis of $(RSC)_6$, carried out over a period of several years, was achieved.....

For typing of headings see section 3.3.6; no underlining (to indicate typography) is called for, as this will be done by the editor.

4.0 Deposition of Data: Supplementary Publications Scheme

Bulk information (such as crystallographic structure factor tables, 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, Lending Division (Boston Spa) (BLLD), 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.

4.1 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.

4.2 Deposition

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

4.3 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 BLLD. The Society will add to the paper a footnote indicating what material has been deposited in the Supplementary Publications Scheme, and the supplementary publication number.

4.4 Availability

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

Mr. J. P. Chillag,
British Libary Lending Division,
Boston Spa,
Wetherby,
West Yorkshire, LS23 7BQ, U.K.

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 papers will be assessed for their chemical as well as their crystallographic 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. Papers reporting only the results of crystal structure determinations will not be accepted for publication unless these results are considered to possess specifically chemical significance.

5.1 Presentation of Crystal Data

The following sequence should be employed (although not all items will be required in all cases): (1) 'molecular' formula and formula weight (M); (2) melting point (m.p.); (3) crystal system; (4) unit cell parameters (translations in Å) and volume of cell (in Å^3); (5) measured density (D_m), no. of molecules in unit cell (Z), and calculated density (D_c); (6) $F(000)$; (7) type(s) of X-rays used, absorption coefficient (μ), and experimental methods; (8) space group and molecular symmetry implied; (9) optical data.

Example: $C_{16}H_{30}BrN_3O_4$, $M = 408.3$, orthorhombic bipyramidal, $a = 7.52(2)$, $b = 18.76(5)$, $c = 27.90(10)$ Å, $U = 3\,936$ Å^3, $D_m = 1.37$ g cm^{-3}, $Z = 8$, $D_c = 1.38$ g cm^{-3}, $F(000)$ 1 712, space group *Pbca* (D_{2h}^{15}, No. 61), Cu-K_α radiation, single-crystal rotation and oscillation photographs.

5.2 Atom Numbering

This should be explained in a graphic formula or in one of the diagrams. If there are differences from the chemical numbering system these 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.* Other symmetry-related atoms can be denoted by primed numerals: C(2′), O(1″), *etc.*; a particular number of primes is to be associated exclusively with a particular asymmetric unit. Alternatively, roman numeral superscripts can be employed: C(2^{I}) . . . C(2^{IV}).

5.3 Atomic Co-ordinates

In giving atomic co-ordinates, authors should state their choice of origin, and it is essential to emphasise the choice when it differs from that adopted in International Tables. For structures in the monoclinic and triclinic systems, it is helpful also to list co-ordinates (in Å) with respect to orthogonal axes, whose orientation to the crystallographic axes should be specified.

5.4 *R*-Values

When citing the R-value authors should state whether unobserved reflections have been included, and if so how. The terms summed in the denominator should be F_o and not F_c. When possible, some estimate of the accuracy of the F_o data ought to be included.

5.5 Structure Factors

Authors must submit along with the manuscript a readable table of structure factors for the referees' inspection. The table should be prepared in accordance with the detail given in section 4.1, so that it may be used for deposition. It must be arranged with the greatest economy of space possible [*i.e.* not less than two groups of columns (h, k, l, F_c, F_o) to the page (30 cm × 21 cm)]. All columns must be headed. A 'paste-up' on white card of computer printout will be acceptable providing the quality of the printout is adequate. If the referees accept the paper the Society will deposit the structure factor tables with the British Library Supplementary Publications Scheme (section 4.1).

5.6 Thermal Parameters

Unless both specifically requested by the author and recommended by the referees for publication, vibrational parameters will be routinely deposited with the structure factors. Where vibrational parameters are to be published they should be in the form of U_{ij} with units of Å^2.

Referees may, at their discretion, recommend other material for deposition where in their view its inclusion in the parent paper is not justified by its interest.

5.7 Diagrams

Each paper should contain a line drawing of the compound under discussion where appropriate in addition to the usual crystallographic figures.

6.0 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 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.