

## Instructions for Authors (1995)

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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 five sections, of which four 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 application of physicochemical techniques to the study of their structures, properties and reactions, including kinetics and mechanisms; new or improved experimental techniques and syntheses.

*Faraday Transactions (Physical Chemistry and Chemical Physics)*. Gas-phase kinetics and dynamics; molecular beam kinetics and spectroscopy; photochemistry and photophysics; energy transfer and relaxation processes; laser-induced chemistry; spectroscopies of molecules, molecular and gas-phase complexes; quantum chemistry and molecular structure, statistical mechanics of gaseous molecules and complexes; spectroscopies, statistical mechanics and quantum theory of the condensed phase, computational chemistry and molecular dynamics; colloid and interface science, surface science, physisorption and chromatographic science, chemisorption and heterogeneous catalysis, zeolites and ion-exchange phenomena; electrode processes, liquids and solutions; solid-state chemistry (microstructures and dynamics); reactions in condensed phases; physical chemistry of macromolecules and polymers; materials science; thermodynamics; biophysical chemistry and radiation chemistry.

*Perkin Transactions 1 (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 2 (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 fifth 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 four *Transactions*) providing detailed accounts of the work.

In addition to full papers, *Dalton Transactions* also publishes Communications and Letters (see sections 6 and 7).

### 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, as a letter to the Editor of some other periodical or as a patent. However, the acceptance of a contribution for *Chemical Communications* or as a *Dalton Communication* does not guarantee that the corresponding full paper will be accepted for *Dalton Transactions*; 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 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 Editorial Manager, Dalton, The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF.

Authors from the USA, Canada and Mexico may address their typescripts to: Professor Gregory S. Girolami, North American Associate Editor, The School of Chemical Sciences, Box 39-1, The University of Illinois at Urbana-Champaign, 505 South Mathews Avenue, Urbana, IL 61801, USA.

Four copies of the typescript (a top copy and three good quality Xerox copies) are required, together with two copies of the crystallographic material for the referees and/or deposition where applicable. For full papers containing material previously published in preliminary form (in whatever journal) then three copies of the preliminary communication are also required. For revised typescripts please supply two copies. Copies of any related, relevant, unpublished material should also be provided. In addition, up to three brief sentences in amplification of the title, for inclusion in the Contents list, should be supplied (see section 3.1.2).

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

On submitting their manuscripts, authors are encouraged to supply the names and addresses of 2–3 potential referees. For a *Dalton Communication* authors should briefly indicate in a covering note or letter the reasons why they feel that rapid publication of their work is justified.

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 in order 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 manuscript is passed for editing. The author receives two copies of proofs, together with the edited manuscript. The Society supplies 50 reprints free of charge.

One corrected proof and the manuscript should be sent to the Editor as soon as possible. Checking of proofs is the authors' 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 summarized in the pamphlet *Authors' alterations cost money and cause delay . . .* which can be purchased from the British Printing Industries Federation (11 Bedford Row, London WC1R 4DX). 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. For the format of Communications and Letters, see sections 6.0 and 7.0.

#### 3.1 Organization of Material

3.1.1 *Title*.—A paper should have a short, straightforward title directed at the general reader. Lengthy systematic names and complicated and numerous chemical formulae should therefore be avoided where possible. The use of abbreviations and symbols in a title is discouraged; terms should be written out in full unless they are extremely cumbersome. Brevity in a title, though desirable, should be balanced against its accuracy and usefulness. Ideally, the title should not occupy more than two lines in the Contents list, see example on p. xvi.

The use of Series titles and Part numbers in titles of papers is discouraged. Instead the Series title and Part number can be included as a footnote to the first page together with a reference (reference 1) to the preceding Part.

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

## Guidelines for submission on disk

These guidelines should be used in conjunction with the *Instructions for Authors* by authors wishing to submit a copy of their manuscript in electronic form. Successful utilisation of data on disk avoids duplication of effort and introduction of typographical error during typesetting/redrawing. The following points should be noted during preparation of the manuscript to allow us to make the best use of the data provided.

**Hardcopy** – copies of the manuscript to be submitted in the usual way

- Submission on disk should accompany the **revised** version of the manuscript, such that **the hardcopy to be edited and the data on the disk are identical**

**Disk** – formatted for IBM (or compatible) PC or Macintosh

- either 3.5 or 5.25"
- clearly labelled (author name, word processor type, file format and file names)
- accompanied on submission with a disk description form

**Data** – *text*: MS-Word, Word for Windows, WordPerfect and WordStar files accepted

- *graphics*: ChemDraw files accepted
- do not integrate text and graphic files**

**Text** – double spaced

- unjustified
- ranged left
- not hyphenated

**Paragraphs** – no indent on first line

- separated by carriage return

**Spaces** – single spaces only after all punctuation, including full point

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

**Tables** – include at the end of the text file

- use **either** the word processor's table editor **or** tabs for formatting, but **not** a mixture of the two

**Graphics** – ChemDraw files submitted on a separate disk

- not to be integrated with text file

**Consistency** – check the manuscript carefully for consistency, particularly in the representation of chemical formulae, compound names and words with alternative spellings

Use of the data supplied, either in whole or in part, cannot be guaranteed. Mathematical equations and tables, in particular, may be re-keyed by the typesetter. Page proofs should be checked in the usual way.

3.1.2 *Amplification of the Title.*—To accompany the title of an article in the Contents list, up to three brief sentences in amplification of the title should be supplied. These will normally be written in the present tense. Suggested examples are shown in the specimen Contents list on p. xvi.

If the article includes a crystal structure determination but this is not indicated in the title, then reference should be made to it in the amplification.

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

*Examples:*

Reaction of  $[\text{Rh}_2(\text{C}_5\text{Me}_5)_2\text{Cl}_4]$  with  $\text{PhC}\equiv\text{CH}$  in acetonitrile in the presence of  $\text{Na}_2\text{CO}_3$  gives two complexes **3** and **4** as well as some isomers of triphenylbenzene and

acetophenone. Complexes **3** and **4** were characterized by  $^{13}\text{C}$  NMR spectroscopy and by single-crystal X-ray structure determinations. Complex **3** has the rhodium  $\pi$ -bonded  $\eta^5$  to a  $\text{C}_5\text{Me}_5$  ring and  $\eta^4$  to the  $\text{C}_4$  ring of a tetraphenylbenzocyclobutene. The benzocyclobutene is very close to planar and only a little distorted upon coordination; the structure of the ligand is best understood in terms of a '1,2-divinylcyclobutadiene' type of bonding. Complex **4** has the rhodium  $\pi$ -bonded  $\eta^5$  to a  $\text{C}_5\text{Me}_5$  ring and  $\eta^4$  to a cyclobutadiene; this cyclobutadiene carries two phenyl substituents (1,3-) and an (unco-ordinated) 6-(1,3,6-triphenylfulvenyl) substituent. Possible routes by which **3** and **4** could be formed are discussed.

Water-soluble manganese(III) porphyrins are oxidised in alkaline aqueous solution to the corresponding manganese(IV) porphyrins which, from magnetic moment measurements, appear to exist in solution as  $\mu$ -oxo-dimers. Midpoint potentials and rate constants for oxidation of the manganese(III) porphyrins have been measured for a series of oxidants and throughout the range  $9 < \text{pH} < 14$ , but the overall electronic charge on the metalloporphyrin had

JOURNAL OF THE CHEMICAL SOCIETY  
**Dalton Transactions**

Inorganic Chemistry

*including bioinorganic, organometallic and solid-state chemistry*

CONTENTS

- 0000 **Bernard F. Hoskins, Christine J. McKenzie, Richard Robson and Lu Zhenrong** **Positively charged Pd<sub>2</sub> complexes of a new thiophenoxide-hinging binucleating ligand: synthesis and crystal structure**
- A Pd<sub>2</sub> complex is synthesised by a Schiff's base condensation; in the product, each palladium atom is co-ordinated by a N<sub>3</sub>(μ-S)Cl ligand set. The crystal structure reveals that two unquestionably inequivalent moieties are bound at the binucleating site.
- 
- 0000 **Paul Brown, Mary F. Mahon and Kieran C. Molloy** **Synthesis, reaction chemistry and crystal structures of sterically hindered tris(trimethylsilyl)methyltin(IV) derivatives**
- Routes have been devised to tin(IV) compounds containing the extremely bulky C(SiMe<sub>3</sub>)<sub>3</sub> group. The X-ray structures are reported for Sn(CH<sub>2</sub>Ph)<sub>2</sub>-[C(SiMe<sub>3</sub>)<sub>3</sub>](OSiMe<sub>3</sub>) and Sn(CH<sub>2</sub>Ph)<sub>2</sub>[C(SiMe<sub>3</sub>)<sub>3</sub>][CH<sub>2</sub>CH=C(SiMe<sub>3</sub>)<sub>2</sub>].
- 
- 0000 **Susan M. Bradley, Ronald A. Kydd and Raghav Yamdagni** **Comparison of the hydrolyses of gallium(III) and aluminium(III) solutions by nuclear magnetic resonance spectroscopy**
- Quantitative <sup>71</sup>Ga NMR measurements show that the hydrolysis of Ga<sup>III</sup> salts follows a course analogous to that for Al<sup>III</sup> salts. Evidence is obtained for the formation of the tridecamer [GaO<sub>4</sub>Ga<sub>12</sub>(OH)<sub>24</sub>(H<sub>2</sub>O)<sub>12</sub>]<sup>7+</sup>.
- 
- 0000 **Brian Beagley, David G. Kelly, Philomena P. MacRory, Charles A. McAuliffe and Robin G. Pritchard** **Rare examples of iron(III) complexes of the SO<sub>2</sub>X ligand, formed by reaction of [FeL<sub>4</sub>X<sub>2</sub>][FeX<sub>4</sub>] (L = OPPh<sub>3</sub> or OAsPh<sub>3</sub>, X = Cl or Br) with sulfur dioxide**
- The course of reaction of [FeL<sub>4</sub>X<sub>2</sub>][FeX<sub>4</sub>] with SO<sub>2</sub> is dependent on the identity of the halide and L, but in most cases yields [FeL<sub>4</sub>{OS(O)X}<sub>2</sub>][FeX<sub>4</sub>]. The oxidation products (PPh<sub>3</sub>O)(PPh<sub>3</sub>OH)(HSO<sub>4</sub>) and (AsPh<sub>3</sub>OH)(HSO<sub>4</sub>) have been isolated following exposure to moist air, and the crystal structure of the latter has been determined.
- 
- 0000 **Neil J. Bailey, John S. Field, Raymond J. Haines and Lesley A. Rix** **Halogenation reactions of electron-rich diphosphazene ligand-bridged derivatives of dicobalt octacarbonyl**
- Halogenation of Co<sub>2</sub>(CO)<sub>4</sub>[μ-(RO)<sub>2</sub>PN(Et)P(OR)<sub>2</sub>]<sub>2</sub> (R = Me or Pr<sup>i</sup>) yields [Co<sub>2</sub>(μ-X)(μ-CO)(CO)<sub>2</sub>{μ-(RO)<sub>2</sub>PN(Et)P(OR)<sub>2</sub>}]<sub>2</sub><sup>+</sup> salts. A crystal structure reveals an A-frame arrangement with one CO and one halogen in the bridging positions. Subsequent rearrangement products include the crystallographically characterised complex with a pendant diphosphazene ligand, [Co(CO)<sub>2</sub>-{P(OMe)<sub>3</sub>}]<sub>2</sub>{(MeO)<sub>2</sub>PN(Et)P(OMe)<sub>2</sub>-κP}[BPh<sub>4</sub>].
- 
- 0000 **Suzuko Yamazaki-Nishida, Yutaka Harima and Kazuo Yamashita** **Generation of anodic and cathodic currents based on photoexcited tris(2,2'-bipyrazine)ruthenium(II) in aqueous solution**
- Anodic and cathodic photocurrents observed with ethylenediaminetetraacetic acid and S<sub>2</sub>O<sub>8</sub><sup>2-</sup> as quenchers are explained in terms of reductive and oxidative quenching of photoexcited [Ru(bipyz)<sub>3</sub>]<sup>2+</sup> (bipyz = 2,2'-bipyrazine), respectively. A theoretical analysis is developed to account for the photocurrents.

little effect upon either parameter. The midpoint potentials for the  $\text{Mn}^{\text{III}}\text{--Mn}^{\text{IV}}$  couple are strongly dependent upon pH and increase with decreasing pH. Although manganese(IV) porphyrins are mild oxidants at pH 14, they should be capable of oxidising water to molecular oxygen in neutral solution. With hypochlorite as oxidant, a second oxidation step is possible and the final product is believed to be a manganese(V) oxoporphyrin.

No summary is required for Letters to *Dalton Transactions*.

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

3.1.5 *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.

3.1.6 *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.

3.1.7 *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.

3.1.8 *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) Descriptions of slight variations of essentially the same technique.

## 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., CD, ESR, GLC, IR, m/m, m.p., NMR, ORD, TLC, UV, UV/VIS, v/v. Other such abbreviations should be defined at first mention, as should abbreviations for ligands, reagents, etc.

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

- (a) A comma is not required before 'and' or 'or' in a series such as 'oxygen, sulfur and selenium' or ' $\lambda_{\text{max}}$ /nm 237, 295 and 343.'
- (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 comma, e.g. (3.9 g, 0.1 mol), (30 cm<sup>3</sup>, 1 mol).

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

(b) In the names of chemical compounds or radicals italics are used for prefixes (other than numerals or symbols) when they define the positions of named substituents, or when they define stereoisomers: other prefixes are printed in roman. (*Note*: Initial capital letters are not to be used with italic prefixes or single-letter prefixes: full stops 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*-bis(glycinato)platinum(II), *gem*- and *vic*-diols, benzil *anti*-oxime.

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

*Note*: Greek letters are not italicised.

3.3.5 *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. and finally (*i*), (*ii*), etc.

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

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

*Examples:*

### Experimental

*Preparation of the Thiolate Complexes*.—(a) Bis(benzenethiolato)bis(dimethyldithiocarbamato)[*N,N*-dimethylhydrazido(2-)]molybdenum(VI) **10**. Benzenethiol (1 g) was added to . . .

*Action of 2-Benzylaminopyridine on  $[\text{Os}_3(\text{CO})_{10}(\text{C}_8\text{H}_{14})_2]$  at 40 °C*.—A solution of the bis(cyclooctene) complex . . .

## 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,

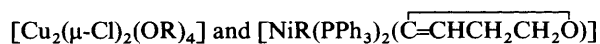
particularly in the form of schemes where the details of a reaction sequence are often more easily understood when illustrated than when described in the text.

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.

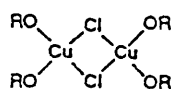
3.4.1 *Structural Formulae*.—(a) Formulae should be numbered with bold arabic numerals (**1**, **2** and **3** etc.)

(b) 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.

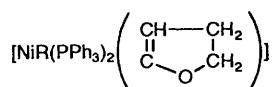
(c) Formulae inserted into the body of the text (as distinct from those displayed separately) should be written on one line if possible, e.g.



rather than



and

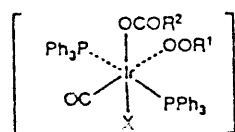


(d) Guidelines for writing linear formulae of complexes are given in *IUPAC Nomenclature of Inorganic Chemistry* (see Section 3.8 of these Instructions). Authors having particular reasons for wishing to deviate from these guidelines should inform the Editor when the paper is submitted.

(e) In formulae of organic ligands 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> and Ph may be used. 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.

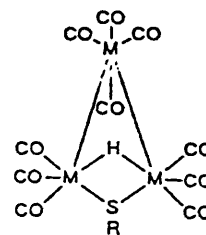
(f) One variable univalent substituent is indicated by R; when more than one independently variable general substituent is

Examples:



	X	R <sup>1</sup>	R <sup>2</sup>
<b>1</b>	Cl	Bu <sup>i</sup>	CF <sub>3</sub>
<b>2</b>	Cl	Bu <sup>i</sup>	CCl <sub>3</sub>
<b>3</b>	Cl	Bu <sup>i</sup>	CHCl <sub>2</sub>
<b>4</b>	Cl	Bu <sup>i</sup>	C <sub>5</sub> F <sub>5</sub>
<b>5</b>	Cl	Bu <sup>i</sup>	CO <sub>2</sub> H
<b>6</b>	Cl	Bu <sup>i</sup>	<i>cis</i> -CH=CHCO <sub>2</sub> H
<b>7</b>	Cl	Bu <sup>i</sup>	H
<b>8</b>	Br	Bu <sup>i</sup>	CF <sub>3</sub>
<b>9</b>	Br	Bu <sup>i</sup>	H
<b>10</b>	Cl	CMe <sub>2</sub> Ph	CF <sub>3</sub>

Examples:



	M	R
<b>1</b>	Ru	[CH <sub>2</sub> ] <sub>3</sub> Si(OMe) <sub>3</sub>
<b>2</b>	Os	[CH <sub>2</sub> ] <sub>3</sub> Si(OMe) <sub>3</sub>
<b>3</b>	Ru	Pr <sup>n</sup>
<b>4</b>	Os	Pr <sup>n</sup>

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. A variable metal may be indicated by M, variable ligands by L<sup>1</sup>, L<sup>2</sup>, etc., and a variable halogen or chalcogen by X.

(g) 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 of alphabetical suffixes (i.e. **1a**, **1b**, **1c** etc.). The use of more than four independently variable substituents or atoms on one generalized formula is discouraged.

(h) 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.

(i) Displayed formulae may be included in tables provided that they can be typed on one line [see point (c) above]; otherwise they should be displayed elsewhere and referred to by number only in the table itself.

(j) 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:

'When the iridium complex **1** was stirred with an excess of iodomethane at room temperature, the adduct **7** was obtained in high yield. The rhodium complexes **4–6** react with iodomethane under similar conditions to give the acetyl complexes **8–10** respectively, formed by isomerization of the first-formed methyl complexes **11–13**.'

(k) 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 *Submission of Structure Diagrams on Disk*.—The Society is willing to receive ChemDraw-produced structure diagrams, reaction schemes, etc., on disk, provided that the data files are supplied in the appropriate format. To facilitate this, the Society will provide, on request, a 3.5" Macintosh diskette containing the preference files and column guides appropriate for producing suitable output with ChemDraw version 2.1.3. Authors wishing to take advantage of this arrangement will be advised to copy these files to their own storage media (diskette or hard disk) for future use. No guarantee can be given that structures produced in this way will be used in the journals as submitted, but it is expected that this route will minimise duplication of the efforts of authors and production staff. To obtain a copy of the diskette, contact Alan McNaught (Manager, Journals) at the Society's Cambridge office.

The preference settings to be used (see below) are as follows: fixed length 0.7 cm; line width 0.025 cm; bold width 0.092 cm;

Preferences		Cancel	Temporary	Permanent
Preferred Units <input type="radio"/> Inches <input checked="" type="radio"/> cm <input type="radio"/> points		Chain Angle <input checked="" type="checkbox"/> degrees		
Fixed Length <input type="text" value="0.7 cm"/>		Bond Spacing <input checked="" type="checkbox"/> % of length		
Bold Width <input type="text" value="0.092 cm"/>	New Captions Font <input type="text" value="Helvetica"/>		Labels Font <input type="text" value="Helvetica"/>	
Line Width <input type="text" value="0.025 cm"/>	Size <input type="text" value="12"/>		Size <input type="text" value="12"/>	
Tolerance <input type="text" value="0.176 cm"/>	<input type="checkbox"/> Bold <input type="checkbox"/> Outline		<input type="checkbox"/> Bold <input type="checkbox"/> Outline	
Margin Width <input type="text" value="0.071 cm"/>	<input type="checkbox"/> Italic <input type="checkbox"/> Shadow		<input type="checkbox"/> Italic <input type="checkbox"/> Shadow	
Hash Spacing <input type="text" value="0.099 cm"/>	<input type="checkbox"/> Underline <input type="checkbox"/> Formula		<input type="checkbox"/> Underline	
		<input checked="" type="checkbox"/> Fractional Character Widths		
		<input checked="" type="checkbox"/> Include Footer <input checked="" type="checkbox"/> PostScript Atom Labels		
		<input checked="" type="checkbox"/> Include ChemDraw Laser Prep in Clipboard		
		<input checked="" type="checkbox"/> Include PostScript commands in Clipboard		
		<input checked="" type="checkbox"/> Fixed Lengths Enabled at Startup		
		<input checked="" type="checkbox"/> Fixed Angles Enabled at Startup		
		<input type="checkbox"/> Show 35mm Slide Boundary Guides		

hash spacing 0.099 cm; bond spacing 20% of width; font Helvetica 12 pt; single width bold and dashed lines should be used to show stereochemistry. Compounds should be numbered with bold arabic numerals and without parentheses (1, 2 and 3, *etc.*). The page set-up for preparation of drawings and printing should be 60%. Single column (8.3 × 22.8 cm) layout is preferred, for flexibility; however, double column (17.1 × 22.8 cm) is acceptable.

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

(b) Figures must be in black ink, on board, white smooth cartridge paper, tracing linen, plastic film (it is essential that the special plastic ink developed for this is used) or graph paper with faint blue lines (red or brown lines must not be present as they 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.

(f) Five-cm margins should be left all round figures. Lettering for insertion at margins should be placed well clear of the ordinate or abscissa line so that it can be copied before erasure.

Lettering and touching-up are done by the Society and clarity of instructions is essential. When there is much lettering, or complicated lettering, and always when tracing linen or plastic film is used, a rough tracing should be provided with the lettering shown in ink.

(g) Since, for printing, the size is reduced, lines should not be too thin. Given lines must be of even thickness, angles neat, and curves smooth. Particular care should be taken with pairs of crystal structure diagrams for stereoscopic viewing: for good reproduction an adequate line thickness is essential.

(h) Graphs should have only the requisite minimum of scale divisions (not less than three points) marked by numerals, and the scale lines should not normally be continued into the body of the figure.

(i) Graphs in any one paper should be drawn to the same scale when convenient, and scale markings should be identical when possible so that the graphs may be placed adjacent on the page. Two curves drawn to different scales can be shown on one graph by having the appropriate scales on the left-hand and the right-hand side. The use of both right- and left-hand axes and

top and bottom axes on figures which have quantitative significance is encouraged.

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

(k) Experimental points must be shown sufficiently large to be distinguishable when reduced in size. Whenever possible, they should be confined to open and closed circles, crosses, squares and triangles. Partly black circles and similar signs frequently become indistinguishable in print.

(l) Curves may be distinguished as full lines (—), broken (---) or dotted lines (···), and dot-dash lines (—·—·—).

(m) For reference in legends, it is preferable to mark curves (a), (b), (c) *etc.* rather than to reproduce the type of line in print.

(n) There must be no unnecessary waste space, *e.g.* around curves; ordinates and abscissae should start at zero only if the curve extends to that range. Enlargements of parts of a figure can occasionally be placed on a corner of the complete figure.

(o) It is not advisable to insert much or complicated lettering on curves or in blank spaces. It is better to label the curves (a), (b), (c) *etc.* and to use explanatory legends.

(p) Large solid objects should be represented by hatching rather than by black surfaces, otherwise the ink may smear on printing.

(q) Photographs are reproduced by a half-tone process. The prints supplied must be very clear and of good contrast, as considerable definition may be lost in reproduction.

(r) 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.

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

### 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.*  $p/\text{atm}$ , or the symbol for a dimensionless physical quantity, *e.g.*  $pV_m^G$ , or some mathematical function of such a number, *e.g.*  $\ln(p/\text{atm})$ .

*Example:*

$\theta/^\circ\text{C}$	$T/\text{K}$	$10^3\text{K}/T$	$p/\text{atm}$	$\ln(p/\text{atm})$	$V_m^G/\text{cm}^3\text{mol}^{-1}$	$pV_m^G/RT$
–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.*  $\frac{V_m^G}{\text{cm}^3\text{mol}^{-1}}$  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, or else presented in tabular form.

The following is suggested as the order in which the most commonly encountered data for a new compound should be cited: yield, melting point, optical rotation, refractive index, elemental analysis, UV absorptions, IR absorptions, NMR spectrum, mass spectrum. Appropriate formats for the citation of each are as follows.

*Yield.* In parentheses after the compound name (or its equivalent). Weight and percentage are separated by a comma, e.g. 'the carbonyl complex (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.

*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, 56.5; H, 4.00.  $C_{12}H_{10}CrO_3$  requires C, 56.7; H, 3.95%). 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, 56.5; H, 4.00. Calc. for  $C_{12}H_{10}CrO_3$ : C, 56.7; H, 3.95%). Analyses are normally quoted to the nearest 0.1%, but a '5' in the second place of decimals is retained.

If a relative molecular mass is to be included, the appropriate form is: [Found: C, 56.5; H, 4.00%;  $M$  (mass spectrum) 254 (or simply  $M^+$  254).  $C_{12}H_{10}CrO_3$  requires C, 56.7; H, 3.95%;  $M$  254].

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

*IR absorptions.* Shown as follows:  $\tilde{\nu}_{max}/cm^{-1}$  2029 and 1955 (CO) and 1714 (NO). The type of signal (s, w, vs) can be indicated by appended letters (e.g. 1760vs).

*NMR 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  $CDCl_3$ ; standard  $SiMe_4$ ) 5.28 [4 H, m,  $J(PtH)$  72 Hz, 4 CH], 2.04 (8 H, s, 4  $CH_2$ ) and 1.80 (30 H, s, 2  $C_5Me_5$ ). 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.  $J(RhP)$  15 Hz,  $J(PH)$  4 Hz, (iv) assignment; underlining for italics can be used to specify the nuclei concerned (e.g.  $CH_3CH_2$ ).

*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  $\tilde{\nu}_{max}/cm^{-1}$  2020 and 1592 (lit.,<sup>24</sup> 2015 and 1600  $cm^{-1}$ ).

*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, and the use of the past tense.

*Synthesis of the Rhodium–Manganese Complex 1.*—Tricarbonyl( $\eta$ -cyclopentadienyl)manganese (0.365 g, 1.79 mmol) in tetrahydrofuran (50  $cm^3$ ) was irradiated (UV) for 2 h at 0 °C under argon. The solution was then treated with  $[Rh(CO)_2(\eta-C_5Me_5)]$  (0.259 g, 0.88 mmol) and the mixture stirred at room temperature for 18 h. Removal of solvent and chromatography afforded unchanged  $[Rh(CO)_2(\eta-C_5Me_5)]$  and  $[Mn(CO)_2(\eta-C_5H_5)]$  followed by yellow-brown crystals of  $[MnRh(\mu-CO)_2(CO)_2(\eta-C_5H_5)(\eta-C_5Me_5)]$  **1** (0.327 g, 79%), m.p. 158–160 °C (Found: C, 48.7; H, 4.5%;  $M^+$  470.  $C_{19}H_{20}MnO_4Rh$  requires C, 48.5; H, 4.3%;  $M$  470);  $\tilde{\nu}_{max}/cm^{-1}$  (CO) 1997(sh), 1991s, 1921vs, 1809w and 1788vs (Nujol); 1983s, 1935vs, 1818w(sh) and 1807s (hexane);  $\delta_H(CDCl_3)$  1.84 (15 H, s,  $C_5Me_5$ ) and 4.62 (5 H, s,  $C_5H_5$ );  $\delta_C(CD_2Cl_2-CH_2Cl_2)$  252.2 [2 C, d,  $J(RhC)$  22 Hz,  $\mu-CO$ ], 227.6 (1 C, s, MnCO), 188.3 [1 C, d,  $J(RhC)$  84 Hz, RhCO], 105.0 ( $C_5Me_5$ ), 86.5 ( $C_5H_5$ ) and 8.9 ( $C_5Me_5$ );  $m/z$  470 ( $M^+$ ), 442 ( $M - CO$ ), 414 ( $M - 2CO$ ), 386 ( $M - 2CO$ ) and 358 ( $M - 4CO$ ).

An example of an alternative, tabular presentation of data is also shown (Table 1).

### 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.

### 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



**Table 1** Analytical<sup>a</sup> and physical data for the platinum–tungsten complexes

Complex	M.p. <sup>b</sup> /°C	Colour	Yield <sup>c</sup> (%)	$\tilde{\nu}(\text{CO})^d/\text{cm}^{-1}$	Analysis (%)	
					C	H
1 [PtW( $\mu$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>3</sub> (PMe <sub>3</sub> )( $\eta$ -C <sub>5</sub> H <sub>5</sub> )]	110–112	Pink	18	2033vs, 1939s, 1865m(sh), 1845m	32.3 (32.3)	3.0 (3.2)
2 [PtW( $\mu$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>3</sub> (PMe <sub>2</sub> Ph)( $\eta$ -C <sub>5</sub> H <sub>5</sub> )]		Red	10	2016s, 1939m, 1843m(br)	37.6 (37.5)	3.2 (3.0)
4 [PtW( $\mu$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>3</sub> (PPh <sub>3</sub> )( $\eta$ -C <sub>5</sub> H <sub>5</sub> ) <sup>e</sup>		Red	40	2027s, 1938s, 1857m(br)		
6 [Pt <sub>2</sub> W( $\mu_3$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>4</sub> (PMe <sub>2</sub> ) <sub>2</sub> ( $\eta$ -C <sub>5</sub> H <sub>5</sub> )]	128–134	Orange	40	2003s, 1989s, 1857m(br), 1763m(br)	26.9 (27.4)	3.4 (3.0)
7 [Pt <sub>2</sub> W( $\mu_3$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>4</sub> (PMe <sub>2</sub> Ph) <sub>2</sub> ( $\eta$ -C <sub>5</sub> H <sub>5</sub> ) <sup>f</sup>	136–140	Orange	41	1993s, 1980s, 1729m	34.3 (34.3)	3.2 (3.0)
8 [Pt <sub>2</sub> W( $\mu_3$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>4</sub> (PMePh <sub>2</sub> ) <sub>2</sub> ( $\eta$ -C <sub>5</sub> H <sub>5</sub> ) <sup>f</sup>	141–145	Dark orange	43	1999vs, 1839s(br), 1746m(br) <sup>g</sup>	40.5 (40.3)	3.2 (3.0)
9 [Pt <sub>2</sub> W( $\mu_3$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>4</sub> (PPh <sub>3</sub> ) <sub>2</sub> ( $\eta$ -C <sub>5</sub> H <sub>5</sub> ) <sup>h</sup>	112–115	Red	27	2003s, 1983s, 1967s, 1923s, 1864m(br), 1784m(br)	48.2 (47.6)	3.6 (3.2)
10 [Pt <sub>2</sub> W( $\mu_3$ -CC <sub>6</sub> H <sub>4</sub> Me-4)(CO) <sub>4</sub> (PEt <sub>3</sub> ) <sub>2</sub> ( $\eta$ -C <sub>5</sub> H <sub>5</sub> )]	160–169	Red	10	1990s, 1829m, 1732m	32.1 (31.9)	3.6 (3.2)

<sup>a</sup> Required values are given in parentheses. <sup>b</sup> With decomposition. <sup>c</sup> Based on tungsten. <sup>d</sup> In methylcyclohexane, unless otherwise stated. <sup>e</sup> Compound not obtained analytically pure due to contamination with PPh<sub>3</sub>. <sup>f</sup> Crystallised with 0.2 molecules CH<sub>2</sub>Cl<sub>2</sub>. <sup>g</sup> In dichloromethane. <sup>h</sup> Crystallised with 0.5 molecule PhMe.

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 reference numbers should be cited in the correct sequence through the text (including those in tables and figure captions, numbered according to where the table or figure is designated to appear). The references themselves are given at the end of the final printed 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,<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).'

**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 xxii and xxiii 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 2000 pages.

If you cannot locate an authoritative abbreviation for a journal, and if it is not obvious how the title should be abbreviated, please cite the full title.

Bibliographic details should be cited in the order: **year, volume, page.**

**Books.** The order of presentation is: author(s), full title (in italics), editor(s), publisher, location, edition, year, volume, chapter and page number(s):

D. Brown, *Halides of the Lanthanides and Actinides*, Wiley, London, 1968, p. 50.

J. Barker, in *Catalyst Deactivation*, eds. B. Delmon and C. Froment, Elsevier, Amsterdam, 2nd edn., 1987, vol. 1, ch. 4, pp. 253–255.

**Patents.** Patents should be indicated in the following form:

*Br. Pat.*, 357 450, 367 455–7. *US. Pat.*, 1 171 230. *Ger. Pat.*, 436 112–4, *Jap. Pat.* 20 101. Dates are indicated thus: *Br. Pat.*, 666 776, 1956. Patents which are applied for must always be given a year, e.g. *Br. Pat.*, Appl. 102, 1982.

*Reports and Bulletins*, etc.

R. A. Allen, D. B. Smith and J. E. Hiscott, *Radioisotope Data*, UKAEA Research Group Report AERE-R 2938, H.M.S.O., London, 1961.

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

*Material presented at meetings.*

R. G. Kidd and H. G. Spinney, presented at the 5th International Conference on Non-Aqueous Solutions, Leeds, 1976.

H. C. Freeman, Proceedings of the 21st International Conference on Coordination Chemistry, Toulouse, 1980.

*Theses.*

A. D. Mount, Ph.D. Thesis, University of London, 1977.

*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., Dalton Trans.*, 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., Dalton Trans.*, in the press (2/01234X).

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

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

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. 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.  
Arzneim.-Forsch.  
Aspects Homogeneous Catal.  
At. Absorb. News.  
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. 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.  
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.  
DEFUZET-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  
Elektrokhimiya  
Endavour  
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.  
Finn Chem. Lett.  
Fiz.-Khim. Mekh. Mater.  
Fiz. Met. Metalloved.  
Flavour Ind.  
Fluorine Chem. Rev.  
Food Manuf.  
Fortschr. Chem. Org. Naturst.  
Fortschr. 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. Vissh. 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  
Hua Hsueh Tung Pao  
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 Spectrum. Ion Processes  
Int. J. Pept. Protein Res.  
Int. J. Quantum Chem.  
Int. J. Quantum Chem., Symp.  
Int. J. Sulfur Chem.  
Int. J. Vitam. Nutr. Res.  
Intra-Sci. Chem. Rep.  
Inz. Chem.  
Ion Exch. Solvent Extr.  
Isr. J. Chem.  
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.  
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. Luminesc.  
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., Polym. Chem. Ed.  
J. Polym. Sci., Polym. Phys. Ed.  
J. Polym. Sci., Polym. Symp.  
J. Prakt. Chem.  
J. Protein Chem.  
J. Quant. Spectrosc. Radiat. Transfer  
J. Radioanal. Nucl. Chem.  
J. Raman Spectrosc.  
J. Res. Inst. Catal., Hokkaido Univ.  
J. Res. Nat. Bur. Stand., Sect. A  
J. Sci. Food Agric.  
J. Sci. Hiroshima Univ., Ser. A2  
J. Sci. Ind. Res.  
J. Soc. 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.  
Kagaku Kogaku  
Kanazawa Daigaku Yakugakubu Kenkyu Nempo  
Kem.-Kemi  
Kem. Tidskr.  
Khim. Geterotsikl. Soedin.  
Khim. Ind. (Sofia)  
Khim. Neft. Mashinost.  
Khim. Prir. Soedin.  
Khim. Promst. (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.  
Langmuir  
Laser Chem.  
Latv. PSR Zinat. Akad. Vestis, Kim. Ser.  
Liebig's Ann. Chem.  
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.

Journal Abbreviations (*continued*)

Mikrochim. Acta	Process Biochem.	Russ. Chem. Rev. (Engl. Transl.)	Transition Met. Chem. (Weinheim, Ger.)
Mol. Cell. Biochem.	Processing	Russ. J. Inorg. Chem. (Engl. Transl.)	Trant. J. Br. Ceram. Soc.
Mol. Cryst. Liq. Cryst.	Proc. Indian Acad. Sci., Sect. A	Russ. J. Phys. Chem. (Engl. Transl.)	Trends Anal. Chem.
Mol. Phys.	Proc. Indian Acad. Sci., Sect. B		Trends Biochem. Sci.
Monaish. Chem.	Proc., K. Ned. Akad. Wet., Ser. B	S. Afr. J. Chem.	Tr. Inst. Elektrokhim., Ural. Nauchn. Tsentr. Akad. Nauk SSSR
Nahrung	Proc. Ned. Akad. Wet., Ser. C	Sankyo Kenkyusho Nempo	
Nat. Prod. Rep.	Proc. Natl. Acad. Sci., India, Sect. A	Sb. Ved. Pr., Vys. Sk. Chemickotechnol., Pardubice	Ukr. Biokhim. Zh.
Nature (London)	Proc. Natl. Acad. Sci. USA	Sch. Sci. Rev.	Ukr. Khim. Zh. (Russ. Ed.)
Naturwissenschaften	Proc. R. Soc. Edinburgh, Sect. A	Schweiz. Apoth.-Ztg.	Usp. Khim.
Neftekhimiya	Proc. R. Soc. London, A	Sci. Cult.	UV Spectrum. Group Bull.
Nippon Kagaku Kaishi	Proc. R. Soc. London, B	Science	Uzb. Khim. Zh.
Nippon Noei Kagaku Kaishi	Proc. Soc. Exp. Biol. Med.	Sci. Pap. Coll. Gen. Educ., Univ. Tokyo	Vestn. Leningr. Univ., Fiz., Khim.
Now. J. Chim.	Prog. Bioorg. Chem.	Sci. Pap. Inst. Phys. Chem. Res. (Jpn.)	Vestn. Mosk. Univ., Ser. 2: Khim.
Nucleosides, Nucleotides	Prog. Colloid Polym. Sci.	Sci. Rep. Res. Inst., Tohoku Univ.	Vestn. Slov. Kem. Drus.
Oesterr. Chem.-Zig.	Prog. Inorg. Chem.	Sci. Rep. Tohoku Univ., Ser. 1	Vestsi Akad. Navuk BSSR. Ser. Khim. Nauk
Online (Weston. Conn.)	Prog. Med. Chem.	Sci. Sinica	Ves:premi Vegyip, Egy. Kozl.
Orbital	Prog. Nucleic Acid Res. Mol. Biol.	Sel. Annu. Rev. Anal. Sci.	Vitam. Horm. (N. Y.)
Organometallics	Prog. Nucl. Magn. Reson. Spectrosc.	Semicond. Insul.	Vopr. Med. Khim.
Org. Magn. Reson.	Prog. Phys. Org. Chem.	Sep. Purif. Methods	Vysokomol. Soedin., Ser. A
Org. Mass. Spectrom.	Prog. React. Kinet.	Sep. Sci. Technol.	Vysokomol. Soedin., Ser. B
Org. Prep. Proced. Int.	Prog. Solid State Chem.	Soap. Cosmet., Chem. Spec.	
Org. React. (N. Y.)	Prog. Surf. Membr. Sci.	Sov. Electrochem. (Engl. Transl.)	Xenobiotica
Org. React. (USSR)	Prog. Surf. Sci.	Sov. J. Bioorg. Chem. (Engl. Transl.)	Yakugaku Zasshi
Org. React. Mech.	Prog. Thin-Layer Chromatogr. Relat. Methods	Sov. J. Coord. Chem. (Engl. Transl.)	Yuki Gosei Kagaku Kyokaiishi
Org. Synth.	Przem. Chem.	Sov. Phys.-Crystallogr. (Engl. Transl.)	
Paint Manuf.	Pure Appl. Chem.	Sov. Radiochem. (Engl. Transl.)	Z. Anorg. Allg. Chem.
Pak. J. Sci.	Pyrethrum Post	Spec. Publ. Chem. Soc.	Zavod. Lab.
Pak. J. Sci. Ind. Res.		Spectrochim. Acta, Part A	Zb. Pr. Chemickotechnol. Fac. SVST
Pak. J. Sci. Res.	Quad. Ing. Chim. Ital.	Spectrochim. Acta, Part B	Z. Chem.
Periodia Polytech., Chem. Eng.	Quim. Nova	Spectrosc. Lett.	Zentralbl. Pharm., Pharmakother. Laboratoriumsdiagn.
Pestic. Sci.		Steroids	Zh. Anal. Khim.
Philos. Mag.	Radiat. Phys. Chem.	Steroids Lipids Res.	Zh. Eksp. Teor. Fiz.
Philos. Trans. R. Soc. London, A	Radiat. Res.	Struct. Bonding (Berlin)	Zh. Evol. Biokhim. Fiziol.
Phosphorus Sulfur	Radiochim. Acta	Stud. Univ. Babes-Bolyai, Chem.	Zh. Fiz. Khim.
Photochem. Photobiol.	Radiokhimiya	Sub-Cell. Biochem.	Zh. Nauchn. Prikl. Fotogr. Kinematogr.
Phys. Chem. Glasses	React. Kinet. Catal. Lett.	Surf. Colloid Sci.	Zh. Neorg. Khim.
Phys. Rev.	Recent Dev. Chem. Nat. Carbon Compd.	Surf. Sci.	Zh. Obsch. Khim.
Phys. Rev. Lett.	Recent Prog. Horm. Res.	Synth. Commun.	Zh. Org. Khim.
Phys. Scr.	Recherches	Synth. Comm.	Zh. Prikl. Khim. (Leningrad)
Phytochemistry	Recl. Trav. Chim. Pays-Bas	Synth. React. Inorg. Metal-Org. Chem.	Zh. Spektrosk.
Pigm. Resin Technol.	Rend. Accad. Sci. Fis. Mat., Naples		Zh. Strukt. Khim.
Pis'ma Zh. Eksp. Teor. Fiz.	Rep. Prog. Appl. Chem.	Taehan Hwahakhoe Chi	Zh. Vses. Khim. Ova im D.I. Mendeleeva
Plast. Polym.	Residue Rev.	Talanta	Z. Kristallogr.
Pol. J. Chem.	Rev. Anal. Chem.	Technol. Rep. Osaka Univ.	Z. Lebensm.-Unters. Forsch.
Polyhedron	Rev. Asoc. Bioquim. Argent.	Theor. Eksp. Khim.	Z. Naturforsch., A
Polym. Age	Rev. Chim. (Bucharest)	Theor. Osn. Khim. Tekhnol.	Z. Naturforsch., B
Polym. Commun.	Rev. Phys. Chem. Jpn.	Tetrahedron	Z. Naturforsch., C
Polymer	Rev. Port. Quim.	Tetrahedron Lett.	Z. Phys. Chem. (Munich)
Polym. Sci. USSR (Engl. Transl.)	Rev. Roum. Biochim.	Text. Res. J.	Z. Phys. Chem. (Leipzig)
Postepy Biochem.	Rev. Roum. Chim.	Theor. Exp. Chem. (Engl. Transl.)	Z. Vitam. Horm., Fermentforsch.
Prikl. Biokhim. Mikrobiol.	Rev. Sci. Instrum.	Thermochim. Acta	Z. Wiss. Photogr., Photophys., Photochem.
Priroda (Moscow)	Rev. Soc. Quim. Mex.	Tin Its Uses	
Proc. Am. Soc. Brew. Chem.	Ric. Sci.	Top. Curr. Chem.	
	Rubber Chem. Technol.	Top. Stereochem.	
		Trans. Inst. Met. Finish.	

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., Dalton Trans.*, 1975, 234.
- 2 A. B. Jones, *J. Chem. Soc., Dalton Trans.*, 1977, 123; 1978, 234.
- 3 A. B. Jones, *J. Chem. Soc., Dalton Trans.*, 1977, 123; *J. Am. Chem. Soc.*, 1956, **78**, 1234.
- 4 A. B. Jones, *J. Chem. Soc.*, 1956, 234; A. B. Jones and C. D. Brown, *J. Chem. Soc. B*, 1967, 234, 1077; 1968, 599.
- 5 A. B. Jones, *J. Am. Chem. Soc.*, 1956, **78**, 1234; A. B. Jones and C. D. Brown, *J. Am. Chem. Soc.*, 1957, **79**, 567; A. B. Jones and E. F. Green, *J. Am. Chem. Soc.*, 1957, **79**, 999.

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

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

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

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

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

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

### 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.

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

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

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

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

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

*Compendium of Chemical Terminology: IUPAC Recommendations*, Blackwell Scientific Publications, 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 International d'Unités' (SI). A detailed treatment is given in the so-called Green Book: *Quantities, Units and Symbols in Physical Chemistry* (Blackwell Scientific Publications, Oxford, 1993 edn.).

*Guidelines for the publications of the Society.* 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 a 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. °C, mmHg, g, h). The derivation of derived non-SI units will be indicated.

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

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

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

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

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

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

**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 <sup>-1</sup>	deci	d	10	deca	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			

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 1000.

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

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

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

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

(7) *Units defined in terms of the best available experimental values of certain physical constants.* These units are not part of the SI. The factors for conversion of these units 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 = 1.66041 × 10 <sup>-27</sup> kg

**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>

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

### 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 pages should be numbered.

The first page should be set out as follows (an example showing part of a first printed page is shown on p. xxvi):

- (i) Name and address for proofs.
- (ii) Title of paper, with capitals for first letter of each noun or adjective only.
- (iii) Up to three brief sentences in amplification of the title.
- (iv) Authors' names; an asterisk should follow the name of the author who is to receive any correspondence.
- (v) 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. For multiple authors at different locations italic superior letters (*a*, *b*, *c* . . . , following the asterisk if present) should be used to identify addresses.

**Table 5** Fractions and multiples of units with special names

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

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

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

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

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

(vii) Main text.

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

For typing of headings see section 3.3.5.

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 can be obtained by individuals both in the UK 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.

## Specimen first page

# Molecular Structures of the Gaseous Dimeric Molecules $\text{Me}_2\text{Ga}(\mu\text{-H})_2\text{GaMe}_2$ and $\text{Me}_2\text{Ga}(\mu\text{-Cl})_2\text{GaMe}_2$ as determined by Electron Diffraction

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The structures of gaseous dimethylgallane and dimethylgallium chloride have been determined by electron diffraction. The results indicate that the predominant vapour species at low pressures and temperatures of 290–350 K are dimeric molecules with diborane-like structures,  $\text{Me}_2\text{Ga}(\mu\text{-X})_2\text{GaMe}_2$  (where X = H or Cl), with heavy-atom skeletons conforming to  $D_{2h}$  symmetry. Salient structural parameters in the  $r_s$  structures are: (i) for  $[\text{Me}_2\text{GaH}]_2$ ,  $r(\text{Ga}\cdots\text{Ga})$  261.0 (0.5),  $r(\text{Ga-C})$  195.4 (0.4) and  $r(\text{Ga-H}_b)$  170.8 (1.4) pm;  $\text{Ga-H}_b\text{-Ga}$  99.6 (1.4) and  $\text{C-Ga-C}$  123.2 (1.5)°; (ii) for  $[\text{Me}_2\text{GaCl}]_2$ ,  $r(\text{Ga}\cdots\text{Ga})$  332.8 (1.9),  $r(\text{Ga-C})$  194.8 (0.3) and  $r(\text{Ga-Cl}_b)$  238.2 (0.4) pm;  $\text{Ga-Cl}_b\text{-Ga}$  88.6 (0.9) and  $\text{C-Ga-C}$  135.4 (2.7)° ('b' denotes a bridging atom). Dimethylgallane thus represents the first gallium hydride containing a  $\text{Ga}(\mu\text{-H})_2\text{Ga}$  bridging unit to be characterised structurally; it is notable for the shortness of the  $\text{Ga}\cdots\text{Ga}$  distance. The two molecules invite structural comparisons with related systems like  $[\text{Me}_2\text{EH}]_2$  (E = B or Al),  $[\text{Me}_2\text{AlCl}]_2$  and  $\text{Ga}_2\text{Cl}_6$ .

## 4.2 Deposition

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

## 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 BLDSC. 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 BLDSC on demand by organizations which are registered borrowers. They should use the normal forms and coupons for such requests addressing them as follows:

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

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

## 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 specific 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

For a paper reporting a crystallographic structure determination it is often appropriate to indicate this information in its title, e.g. by the words 'crystal structure of,' but this is not obligatory. However if the crystal structure determination is not indicated in the title then reference should be made to it in the amplification (see section 3.1.2).

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 ( $D_c$ ) (with any implications for 'molecular symmetry'); (7) value of  $F(000)$ ; (8) colour, size and shape of crystal used for data collection; (9) 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  $R'$  (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) For triclinic cells the Niggli reduced cell should be reported.

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

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

(7) 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,  $\beta = 91.03(3)^\circ$ ,  $U = 4480$  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),  $Z = 4$ ,  $D_c = 1.76$  g cm<sup>-3</sup>,  $F(000) = 2160$ . 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,  $\mu(\text{Mo-K}\alpha) = 85.12$  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  $1.3$ – $6.8^\circ$  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  $U_{\text{iso}}$  [=  $0.08(2)$  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  $R'$  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 preparation 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 coordinates (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) coordinates should refer to atoms which are all in the same molecule. Hydrogen atom coordinates 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>). The symmetry operation that relates the asymmetric unit to which the primes or superscripts refer, to the asymmetric unit used in the table of coordinates, should be clearly specified.

5.6.2 *For the Referees and/or for Deposition.*—Two copies of:

(1) A table of final fractional atomic coordinates.

(2) Any calculated coordinates (e.g. hydrogen).

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

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

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

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

5.6.3 *Deposition of Material at the Cambridge Crystallographic Data Centre.*—The table of final fractional atomic coordinates, the full list of bond lengths and angles and the list of thermal parameters will be deposited at the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ

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

(or at the Fachinformationszentrum Karlsruhe, Gesellschaft für wissenschaftlich-technische Informationen, D-76344 Eggenstein-Leopoldshafen, Germany, via Dr. P. Luksch, for molecules not containing 'organic' carbon). The material for deposition should include a completed abstract form for each crystallographic determination (a blank for photocopying is reproduced at the end of these Instructions). All tables should be of publication quality. Computer printout is acceptable provided that it is clearly legible. The print program used should yield concise tables of atomic and other derived parameters. The content of the tables should be non-redundant, and their interpretation immediately obvious. The thermal parameters should be submitted as separate tables, with clear definition of the units used. Any request to Cambridge or to the Fachinformationszentrum Karlsruhe for deposited material should be accompanied by the full literature citation for the paper concerned.

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

### 5.7 Reference to Crystallographic Work Published in a Preliminary Communication

It is permissible to regard a fully refined crystal structure determination published in *Chemical Communications* or as a *Dalton Communication* 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 *in full* 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 coordinates *etc.* will be deposited at the Cambridge Crystallographic Data Centre (or the Fachinformationszentrum Karlsruhe). The brief published description of the determination should be supplemented by appropriate reference to 'unpublished work'.

### 6.0 Dalton Communications

Preliminary accounts of original and significant work of such importance that rapid publication is justified may be published in *Communication* form. Material intended for *Dalton Communications* should be of specific specialist interest to inorganic chemists, while work of wide general appeal is more appropriate for submission to *Chemical Communications*. Brief details of key experiments are permitted, but extensive spectroscopic and other supporting data are not required; authors are encouraged to supply such data as supplementary information to aid the referees in their assessment of the work.

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 provided that they represent a substantial amplification and extension of the original material.

Individual articles should be as brief as possible, and not exceed two printed pages (5–6 pages of typescript, including tables, figures, *etc.*). The length of the summary is restricted to one sentence only. For those *Communications* containing crystal structure determinations the atomic coordinates will not be published; crystal data should be incorporated in a footnote and selected molecular dimensions contained within figure captions. The full data will be deposited at the Cambridge Crystallographic Data Centre. Otherwise the format and style of presentation is the same as for a full paper.

Times to publication will be similar to *Chemical Communications*. In order to achieve this, failure of an author to supply a revised script in response to referees' comments within 2 weeks may be regarded as withdrawal of the *Communication*. Furthermore, proof corrections received more than 1 week after despatch of the proofs may not be incorporated.

### 7.0 Letters

Letters, published only in *Dalton Transactions*, are a medium for the expression/exchange of scientific opinions/views normally concerning material published in *Dalton Transactions*, but not for revision/updates of authors' own work. They are not intended to compete with media for the publication of more general matters such as *Chemistry in Britain*.

Only rarely should a Letter exceed one printed column in length (about 1–2 pages of typescript). Where a Letter is polemical in nature, and if it is accepted, a Reply will be solicited from other parties implicated for publication alongside the original Letter.

### 8.0 Publication of Theoretical and Computational Papers

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

(i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to *Faraday Transactions*, one in which the computations are incidental to the chemistry to *Perkin, Dalton* or *Faraday Transactions*. Papers concerned mainly with computational details are unlikely to be accepted.

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

(iii) Many papers use a routine procedure based on a well documented method, be it 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 the 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.

## 9.0 Molecular Modelling Guidelines

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

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

(b) A concise indication in a 'Computational Details Section' or a footnote of standard options involved such as basis sets, SCF methods, electronic states, parameter sets, charge distribution schemes, symmetry, geometry optimisation methods, convergence criteria, cut-offs, time constants, *etc.* More explicit details of any non-standard use of *e.g.* basis sets, force-field parameters, algorithmic options, *etc.* should be particularly provided.

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

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

## 10.0 Publication of Stability Constant Measurements

Authors should provide sufficient information to enable the reader to establish quickly and unambiguously the exact conditions used, and also to evaluate properly the experimental results.

Information appropriate to the following requirements should therefore appear in any paper reporting stability constant measurements.

- 1 The purity of reagents and solvents, and the procedures followed in solvent or reagent purification.
- 2 The composition of the solution, especially the ionic strength, and any other relevant factors including the range of metal and ligand concentrations investigated. For mixed solvent systems, the solvent composition must be defined.
- 3 When appropriate, the pH range over which measurements have been made, the titrant used, and the  $K_w$  value assumed.
- 4 The instrument(s) (*e.g.*, pH meter, electrode, spectrophotometer, *etc.*) used in the experimental studies, and an explicit description of the method of calibration.
- 5 The temperature and temperature range.

**Table** Summary of experimental parameters for the system copper(II)-tyrosyl-glycyl-prolyl-tyrosine

Solution composition	
$[T_L]$ range/mol dm <sup>-3</sup>	0.003–0.005
$[T_M]$ range/mol dm <sup>-3</sup>	0.001–0.004
$I$ /mol dm <sup>-3</sup> , electrolyte	0.010, KNO <sub>3</sub>
pH Range	2.7–10.8 (protonation)
Experimental method	pH Titration, calibrated in concentrations
$T/^\circ\text{C}$	25
Total number of data points	
Protonation	207 (2 titrations)
Copper complexation	274 (3 titrations)
Method of calculation	SUPERQUAD <sup>reference</sup>
Protonation constants (ligand = H <sub>3</sub> L, errors as $\sigma$ )	
log $\beta_{HL}$	10.16 $\pm$ 0.01
log $\beta_{H_2L}$	19.96 $\pm$ 0.01
log $\beta_{H_3L}$	27.50 $\pm$ 0.02
log $\beta_{H_4L}$	30.52 $\pm$ 0.03
Stability constants	
log $\beta_{CuL}$	10.29 $\pm$ 0.09
log $\beta_{CuHL}$	19.70 $\pm$ 0.01
log $\beta_{CuH_2L}$	24.36 $\pm$ 0.05
log $\beta_{Cu_2L_2}$	24.00 $\pm$ 0.05
log $\beta_{Cu_2H_2L_2}$	3.66 $\pm$ 0.02

6 The number of data points recorded in a titration (or elsewhere as appropriate), and the number of replicate measurements.

7 The computer program, or any other method of calculation used to derive final results from the experimental values, and a literature reference if the programs are the work of others; new programs should be shown in terms of the stepwise logic involved. Any discussion of the reasons for choosing a given program may form an appropriate part of the text of the paper.

8 The range of the results, the standard deviation of the final result, the sources of error, and the methods used in establishing these parameters.

This may be presented in tabular form (see example) and any special comments placed in the text. It is also recommended that protonation constants (log  $\beta_{HL}$  *etc.*) and stability constants (log  $\beta_{CuHL}$ , log  $\beta_{222}$  *etc.*) be defined (see *IUPAC Compendium of Analytical Nomenclature, Definitive Rules 1987*, eds. H. Freiser and G. H. Nancollas, Blackwell Scientific Publications, Oxford, 1987, pp. 9–15).

Finally, it is suggested that some discussion of the reasons which prompted the experiments, and of the chemical information which has subsequently been derived from the measurements, would serve to make stability constant data an intrinsic part of chemistry as a whole, rather than a separate and sometimes esoteric field in itself. Similarly, comparisons with previous determinations on identical or similar metal–ligand systems would help to place the work in context.

**CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM**

Compound Name
Diagram ( <i>conventional chemical structural diagram</i> )
Formula ( <i>each residue to be formulated ,eg. C<sub>2</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup> · Na<sup>+</sup> · 2H<sub>2</sub>O</i> )

<i>a</i> (Å) with estimated error		<i>b</i> (Å) with estimated error		<i>c</i> (Å) with estimated error	
alpha(deg.)with estimated error		beta(deg.) with estimated error		gamma(deg.) with estimated error	
Space Group	Z	R-factor(s) R	Temp(K)	Radiation <input type="checkbox"/> X <input type="checkbox"/> N	Powder Data Yes <input type="checkbox"/> No <input type="checkbox"/>
Intensity Measurement <input type="checkbox"/> densit. <input type="checkbox"/> diffr. <input type="checkbox"/> other( <i>specify</i> )			Volume(Å <sup>3</sup> )	Mol. Weight	Mp(°C)
Absolute Configuration Determined <input type="checkbox"/> Yes <input type="checkbox"/> No		Colour  CAS RN		D <sub>m</sub> (g cm <sup>-3</sup> )  D <sub>x</sub> (g cm <sup>-3</sup> )	
Polymorph Indicator ( <i>eg. low-temp. form</i> )					
Drug ( <i>indicate, where appropriate, type of drug, activity, etc.</i> )					
Disorder ( <i>specify nature of disorder with reference to atom labels in coordinate list</i> )					

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## APPENDIX

***IUPAC Publications on Nomenclature and Symbolism*****1.0 Compilations**

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

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

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

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

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

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

- Nomenclature of organic chemistry. Section E: Stereochemistry (1974)
- Nomenclature of organic chemistry. Section F: Natural products and related compounds (1976)
- Isotopically modified compounds
- Recommendations for the presentation of thermodynamic and related data in biology (1985)
- Citation of bibliographic references in biochemical journals (1971)
- Nomenclature and symbolism for amino acids and peptides (1983)
- Abbreviated nomenclature of synthetic polypeptides or polymerized amino acids (1971)
- Abbreviations and symbols for the description of the conformation of polypeptide chains (1969)
- Nomenclature of peptide hormones (1974)
- Nomenclature of glycoproteins, glycopeptides and peptidoglycans (1985)
- Nomenclature of initiation, elongation and termination factors for translation in eukaryotes (1988)
- Nomenclature of multiple forms of enzymes (1976)

- Symbolism and terminology in enzyme kinetics (1981)
- Nomenclature for multienzymes (1989)
- Abbreviations and symbols for nucleic acids, polynucleotides and their constituents (1970)
- Abbreviations and symbols for the description of the conformations of polynucleotide chains (1982)
- Nomenclature for incompletely specified bases in nucleic acid sequences (1984)
- Carbohydrate nomenclature. Part I (1969)
- Nomenclature of cyclitols (1973)
- Numbering of atoms in *myo*-inositol (1988)
- Conformational nomenclature for five- and six-membered ring forms of monosaccharides and their derivatives (1980)
- Nomenclature of unsaturated monosaccharides (1980)
- Nomenclature of branched-chain monosaccharides (1980)
- Abbreviated terminology of oligosaccharide chains (1980)
- Polysaccharide nomenclature (1980)
- Symbols for specifying the conformation of polysaccharide chains (1981)
- Nomenclature of lipids (1976)
- Nomenclature of steroids (1989)
- Nomenclature of quinones with isoprenoid side chains (1973)
- Nomenclature of carotenoids (1970) and amendments (1974)
- Nomenclature of tocopherols and related compounds (1981)
- Nomenclature of vitamin D (1981)
- Nomenclature of retinoids (1981)
- Prenol nomenclature (1986)
- Nomenclature of phosphorus-containing compounds of biochemical importance (1976)
- Nomenclature and symbols for folic acids and related compounds (1986)
- Nomenclature for vitamins B-6 and related compounds (1973)
- Nomenclature of corrinoids (1973)
- Nomenclature of tetrapyrroles (1986)

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

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

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

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

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

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

## 2.0 Documents not included in the compilations

### 2.1 Nomenclature of Elements and Compounds

#### *Boron Compounds*

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

#### *Delta Convention*

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

#### *Elements*

Recommendations for the names of elements of atomic number greater than 100 (*Pure Appl. Chem.*, 1979, **51**, 381).

#### *Enzymes*

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

#### *Heterocyclic Compounds*

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

#### *Hydrogen*

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

#### *Isotopically Modified Compounds*

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

#### *Lambda Convention*

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

#### *Nitrogen Hydrides*

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

#### *Numerical Terms*

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

#### *Polyanions*

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

#### *Polymers*

Nomenclature of regular double-strand (ladder and spiro) organic polymers (*Pure Appl. Chem.*, 1993, **65**, 1561).  
Structure-based nomenclature for irregular single-strand organic polymers (*Pure Appl. Chem.*, 1994, **66**, 873).

#### *Radicals and Ions*

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

#### *Zeolites*

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

## 2.2 Terminology, Symbols and Units, and Presentation of Results

### *General*

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

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

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

### *Analytical*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

### *Biotechnology*

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

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

### *Clinical*

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

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

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

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

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

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

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

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

#### *Colloids and Surface Chemistry*

Definitions, terminology and symbols in colloid and surface chemistry. I (*Pure Appl. Chem.*, 1972, **31**, 577). II, Heterogeneous catalysis (*Pure Appl. Chem.*, 1976, **46**, 71). Part 1.14: Light scattering (provisional) (*Pure Appl. Chem.*, 1983, **55**, 931). Reporting experimental pressure–area data with film balances (*Pure Appl. Chem.*, 1985, **57**, 621).

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

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

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

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

#### *Electrochemistry*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

#### *Kinetics*

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

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

#### *Photochemistry*

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

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

#### *Quantum Chemistry*

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

#### *Reactions*

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

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

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

#### *Rheological Properties*

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

#### *Spectroscopy*

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

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

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

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

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

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

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

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

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

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

Nomenclature, symbols, units and their usage in spectrochemical analysis. VII. Molecular absorption spectroscopy, UV and visible (*Pure Appl. Chem.*, 1988, **60**, 1449); VIII.

Nomenclature system for X-ray spectroscopy (*Pure Appl. Chem.*, 1991, **63**, 735); X. Preparation of materials for analytical atomic spectroscopy (*Pure Appl. Chem.*, 1988, **60**, 1461); XII.

Terms related to electrothermal atomization (*Pure Appl. Chem.*, 1992, **64**, 253); XIII. Terms related to chemical vapour generation (*Pure Appl. Chem.*, 1992, **64**, 261).

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

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

#### *Solid State*

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

#### *Thermodynamics*

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

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

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

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

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

#### *Toxicology*

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