JOURNAL OF THE CHEMICAL SOCIETY, DALTON TRANSACTIONS

Instructions for Authors (1994)

CONTENTS

1.0 General Policy

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

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

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

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, if requested, execute a formal licence granting the Society exclusive licence under any copyright therein.

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

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

1.2 Submission of Articles

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

Four copies of the typescript (a top copy and three good quality carbon or 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).

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 and reprint order form. The Society supplies 50 reprints free of charge, and further copies can be purchased.

One corrected proof *and* the manuscript, the reprint order form, and payment (if any) should be sent to the Editor 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

---

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

91. (iii) Every member who submits a paper or other communication with a view to its publication by the Society shall by so doing undertake: (*a*) that his communication has not been published and that he will not permit its publication before it is accepted or declined by the Society, and

(*b*) that if it is accepted for publication the Society shall thereupon become entitled to an exclusive licence under any copyright therein (which shall include the right to sublicence) and that he will, if then called upon to do so, execute a formal licence to the Society of the said copyright, including the sole right to publish in any form in any language and in any part of the world, the whole or any part of his communication. The Council shall not refuse any reasonable request from an author to reproduce his own work elsewhere in whole or in part.

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

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

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. xiv.

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

> Metal Complexes of Benzodiazepines. Part 2.[1] Reaction of 1,4-Benzodiazepines with Halide-bridged Complexes of Palladium(II) $[Pd_2X_4(PPr_3)_2]$ (X = Cl or I).

The corresponding reference should be in the form:

> 1 Part 1, M. C. Aversa, P. Giannetto, G. Bruno, M. Cusumano, A. Giannetto and S. Geremia, *J. Chem. Soc., Dalton Trans.*, 1990, 2433.

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

3.1.2 *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. xiv.

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 $[Rh_2(C_5Me_5)_2Cl_4]$ with PhC≡CH in acetonitrile in the presence of Na_2CO_3 gives two complexes **3** and **4** as well as some isomers of triphenylbenzene and acetophenone. Complexes **3** and **4** were characterized by ^{13}C NMR spectroscopy and by single-crystal X-ray structure determinations. Complex **3** has the rhodium π-bonded η^5 to a C_5Me_5 ring and η^4 to the C_4 ring of a tetraphenylbenzocyclobutene. The benzocyclobutene is very close to planar and only a little distorted upon co-ordination; the structure of the ligand is best understood in terms of a '1,2-divinylcyclobutadiene' type of bonding. Complex **4** has the rhodium π-bonded η^5 to a C_5Me_5 ring and η^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 μ-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 $9 < pH < 14$, but the overall electronic charge on the metalloporphyrin had little effect upon either parameter. The midpoint potentials for the Mn^{III}–Mn^{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 'λ_{max}/nm 237, 295 and 343.'

Specimen Contents List

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_2 complexes of a new thiophenoxide-hinging binucleating ligand: synthesis and crystal structure

A Pd_2 complex is synthesised by a Schiff's base condensation; in the product, each palladium atom is co-ordinated by a $N_3(\mu\text{-}S)Cl$ 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 $C(SiMe_3)_3$ group. The X-ray structures are reported for $Sn(CH_2Ph)_2[C(SiMe_3)_3](OSiMe_3)$ and $Sn(CH_2Ph)_2[C(SiMe_3)_3][CH_2CH{=}C(SiMe_3)_2]$.

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 ^{71}Ga NMR measurements show that the hydrolysis of Ga^{III} salts follows a course analogous to that for Al^{III} salts. Evidence is obtained for the formation of the tridecamer $[GaO_4Ga_{12}(OH)_{24}(H_2O)_{12}]^{7+}$.

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_2X ligand, formed by reaction of $[FeL_4X_2][FeX_4]$ (L = $OPPh_3$ or $OAsPh_3$, X = Cl or Br) with sulfur dioxide

The course of reaction of $[FeL_4X_2][FeX_4]$ with SO_2 is dependent on the identity of the halide and L, but in most cases yields $[FeL_4\{OS(O)X\}_2][FeX_4]$. The oxidation products $(PPh_3O)(PPh_3OH)(HSO_4)$ and $(AsPh_3OH)(HSO_4)$ 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 $Co_2(CO)_4[\mu\text{-}(RO)_2PN(Et)P(OR)_2]_2$ (R = Me or Pr^i) yields $[Co_2(\mu\text{-}X)(\mu\text{-}CO)(CO)_2\{\mu\text{-}(RO)_2PN(Et)P(OR)_2\}_2]^+$ 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, $[Co(CO)_2\{P(OMe)_3\}_2\{(MeO)_2PN(Et)P(OMe)_2\text{-}\kappa P\}][BPh_4]$.

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 $S_2O_8^{2-}$ as quenchers are explained in terms of reductive and oxidative quenching of photoexcited $[Ru(bipyz)_3]^{2+}$ (bipyz = 2,2′-bipyrazine), respectively. A theoretical analysis is developed to account for the photocurrents.

(*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^3, 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* $[Os_3(CO)_{10}(C_8H_{14})_2]$ *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.

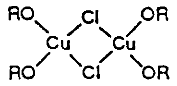
3.4.1 *Structural Formulae.*—(*a*) Formulae should be numbered with bold arabic numerals (**1**, **2** and **3** *etc.*)

(*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.

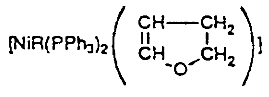
(*c*) Formulae inserted into the body of the text (as distinct from those displayed separately) should be written on one line if possible, *e.g.*

$[Cu_2(\mu\text{-}Cl)_2(OR)_4]$ and $[NiR(PPh_3)_2(\overline{CH{=}CHCH_2CH_2O})]$

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^n, Pr^i, Bu^n, Bu^i Bu^s, Bu^t and Ph may be used. Other special symbols, if used, require an explanatory footnote. The carboxy-group is written CO_2H (not COOH); similarly CO_2R.

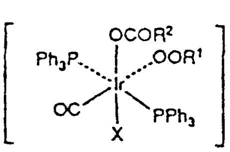
(*f*) One variable univalent substituent is indicated by R; when more than one independently variable general substituent is present, R^1, R^2 and R^3 should be used not R, R^1, R^2, R^3; or R_1, R_2 and R_3, which indicate 1 × R, 2 × R, *etc.* A variable metal may be indicated by M, variable ligands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

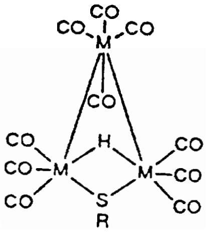
(*i*) Displayed formulae may be included in tables provided

Examples:



	X	R^1	R^2
1	Cl	Bu^t	CF_3
2	Cl	Bu^t	CCl_3
3	Cl	Bu^t	$CHCl_2$
4	Cl	Bu^t	C_5F_5
5	Cl	Bu^t	CO_2H
6	Cl	Bu^t	*cis*-$CH{=}CHCO_2H$
7	Cl	Bu^t	H
8	Br	Bu^t	CF_3
9	Br	Bu^t	H
10	Cl	CMe_2Ph	CF_3

Examples:



	M	R
1	Ru	$[CH_2]_3Si(OMe)_3$
2	Os	$[CH_2]_3Si(OMe)_3$
3	Ru	Pr^n
4	Os	Pr^n

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.

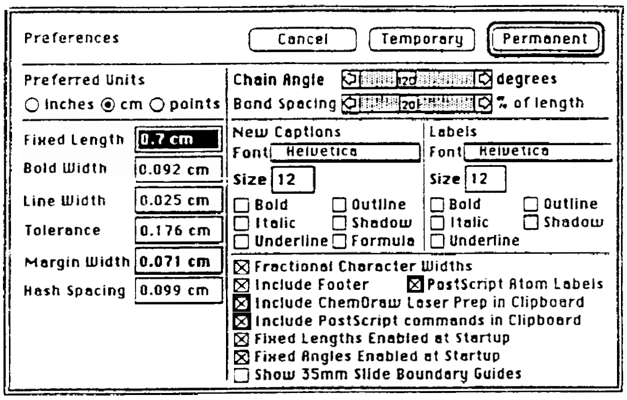
(*j*) The key number for a compound may be used in the cursive text to avoid repetition of long chemical names; this device must not be used to excess. In general it is preferred if the key number is qualified by a partial name as in the following example:

'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; 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.



Preferred Units
○ Inches ● cm ○ points

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

Chain Angle 120 degrees
Bond Spacing 20 % of length

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

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

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

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/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/atm).

Example:

θ/°C	T/K	10^3K/T	p/atm	ln(p/atm)	V_m^G/cm^3 mol^{-1}	pV_m^G/RT
−51.60	216.55	4.6179	5.112	1.6316	3 177.6	0.9142

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

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

3.5.2 *Physical Characteristics of Compounds.*—Data associated with particular compounds should be listed after the name of the compound concerned, following the description of its preparation, 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 λ_{max}/nm (EtOH) 228 (ε/dm^3 mol^{-1} cm^{-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: λ_{max}/nm (EtOH) 228, 262 and 302 (ε/dm^3 mol^{-1} cm^{-1} 40 900, 19 200 and 11 500). Log ε may be quoted instead of ε.

IR absorptions. Shown as follows: $\tilde{\nu}_{max}$/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 δ values should be used, with the nucleus indicated by subscript if necessary (*e.g.* δ_H, δ_C). Instrument frequency, solvent and standard should be specified. For example: δ_H(100 MHz; solvent $CDCl_3$; standard $SiMe_4$) 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.* $CH_3C\mathit{H}_2$).

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 ($189 \longrightarrow 174$), 147 ($176 \longrightarrow 161$), *etc.* The type of spectrum (field desorption, electron impact, *etc.*) should be indicated.

Literature citations. If comparison is to be made with literature values, these should be quoted in parentheses, *e.g.* m.p. 157 °C (from chloroform) (lit.,[19] 156 °C), or $\tilde{\nu}_{max}$/cm^{-1} 2020 and 1592 (lit.,[24] 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(η-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); δ_H($CDCl_3$) 1.84 (15 H, s,

Table 1 Analytical[a] and physical data for the platinum–tungsten complexes

Complex	M.p.[b]/°C	Colour	Yield[c] (%)	$\tilde{\nu}(CO)$[d]/cm^{-1}	Analysis (%)	
					C	H
1 $[PtW(\mu\text{-}CC_6H_4Me\text{-}4)(CO)_3(PMe_3)(\eta\text{-}C_5H_5)]$	110–112	Pink	18	2033vs, 1939s, 1865m(sh), 1845m	32.3 (32.3)	3.0 (3.2)
2 $[PtW(\mu\text{-}CC_6H_4Me\text{-}4)(CO)_3(PMe_2Ph)(\eta\text{-}C_5H_5)]$		Red	10	2016s, 1939m, 1843m(br)	37.6 (37.5)	3.2 (3.0)
4 $[PtW(\mu\text{-}CC_6H_4Me\text{-}4)(CO)_3(PPh_3)(\eta\text{-}C_5H_5)]$[e]		Red	40	2027s, 1938s, 1857m(br)		
6 $[Pt_2W(\mu_3\text{-}CC_6H_4Me\text{-}4)(CO)_4(PMe_3)_2(\eta\text{-}C_5H_5)]$	128–134	Orange	40	2003s, 1989s, 1857m(br), 1763m(br)	26.9 (27.4)	3.4 (3.0)
7 $[Pt_2W(\mu_3\text{-}CC_6H_4Me\text{-}4)(CO)_4(PMe_2Ph)_2(\eta\text{-}C_5H_5)]$[f]	136–140	Orange	41	1993s, 1980s, 1729m	34.3 (34.3)	3.2 (3.0)
8 $[Pt_2W(\mu_3\text{-}CC_6H_4Me\text{-}4)(CO)_4(PMePh_2)_2(\eta\text{-}C_5H_5)]$[f]	141–145	Dark orange	43	1999vs, 1839s(br), 1746m(br)[g]	40.5 (40.3)	3.2 (3.0)
9 $[Pt_2W(\mu_3\text{-}CC_6H_4Me\text{-}4)(CO)_4(PPh_3)_2(\eta\text{-}C_5H_5)]$[h]	112–115	Red	27	2003s, 1983s, 1967s, 1923s, 1864m(br), 1784m(br)	48.2 (47.6)	3.6 (3.2)
10 $[Pt_2W(\mu_3\text{-}CC_6H_4Me\text{-}4)(CO)_4(PEt_3)_2(\eta\text{-}C_5H_5)]$	160–169	Red	10	1990s, 1829m, 1732m	32.1 (31.9)	3.6 (3.2)

[a] Required values are given in parentheses. [b] With decomposition. [c] Based on tungsten. [d] In methylcyclohexane, unless otherwise stated. [e] Compound not obtained analytically pure due to contamination with PPh_3. [f] Crystallised with 0.2 molecules CH_2Cl_2. [g] In dichloromethane. [h] Crystallised with 0.5 molecule PhMe.

> C_5Me_5) and 4.62 (5 H, s, C_5H_5); $\delta_C(CD_2Cl_2\text{–}CH_2Cl_2)$ 252.2 [2 C, d, J(RhC) 22 Hz, μ-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 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,[3] which . . .'.

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

Journals. The style of journal abbreviations to be used in the Society's publications is that defined in Chemical Abstracts Service Source Index (CASSI). The abbreviations listed in CASSI are based upon internationally recognised systems. The list of CASSI-style abbreviations on pages xix and xx 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.**

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
AIChE J.
Ambix
Am. J. Pharm.
Am. J. Sci.
An. Acad. Bras. Cienc.
Anal. Biochem.
Anal. Chem.
Anal. Chim. Acta
Anal. Lett.
Analusis
Analyst (London)
An. Bromatol.
Angew. Chem.
Angew. Chem., Int. Ed. Engl.
Angew. Makromol. Chem.
Ann. Acad. Sci. Fenn., 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. Absorbt. Newsl.
Aust. J. Biol. Sci.
Aust. J. Chem.
Aust. J. Phys.
Azerb. Khim. Zh.

Ber. Bunsenges. Phys. Chem.
Biochem. Biophys. Res. Commun.
Biochem. Educ.
Biochemistry
Biochemistry (Eng. Transl.)
Biochem. J.
Biochem. Pharmacol.
Biochem. Prep.
Biochem. Soc. Trans.
Biochim. Biophys. Acta
Biochimie
Biofizika
Bioinorg. Chem.
Biokhimiya
Bioorg. Chem.
Bioorg. Khim.
Biopolymers
Biotechnol. Bioeng.
Bochu-Kagaku
Boll. Soc. Ital. Biol. Sper.
Br. Corros. J.
Br. J. Pharmacol.
Br. Polym. J.
Bul. 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.

DEFAZET-Dtsch. Farben-Z.
Denki Kagaku yobi Kogyo Butsuri Kagaku
Dokl. Akad. Nauk Arm. SSR
Dokl. Akad. Nauk SSSR
Dokl. Bolg. Akad. Nauk
Dokl. Chem. (Engl. Transl.)
Dokl. Chem. Technol. (Engl. Transl.)
Dokl. Phys. Chem. (Engl. Transl.)
Dopov. Akad. Nauk Ukr. RSR, Ser. B
Double-Liaison
Dtsch. Lebensm.-Rundsch.
Dyn. Mass Spectrom.

Educ. Chem.
Egypt. J. Chem.
Electroanal. Chem.
Electrochim. Acta
Elektrokhimiya
Endeavour
Environ. Sci. Technol.
Erdoel Kohle, Erdgas, Petrochem., Brennst. Chem.
Essays Biochem.
Eur. J. Biochem.
Eur. Polym. J.
Experientia
Faraday Discuss. Chem. Soc.
Faraday Symp. Chem. Soc.
FEBS Lett.
Fermentn, Spirt. Prom.
Fette, Seifen. Anstrichm.
Finn Chem. Lett.
Fiz.-Khim. Mekh. Mater.
Fiz. Met. Metalloved.
Flavour Ind.
Fluorine Chem. Rev.
Food Manuf.
Fortschr. Chem. Org. Naturst.
Fortschr. Hochpolym.-Forsch.
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 Turkm. SSR, Ser. Fiz.-Tekh., Khim. Geol. Nauk
Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk

J. Agric. Food Chem.
J. Am. Chem. Soc.
J. Am. Leather Chem. Assoc.
J. Am. Oil Chem. Soc.
J. Anal. At. Spectrom.
J. Anal. Chem. USSR (Engl. Transl.)
J. Appl. Chem. Biotechnol.
J. Appl. Chem. USSR (Engl. Transl.)
J. Appl. Crystallogr.
J. Appl. Polym. Sci.
J. Assoc. Off. Anal. Chem.
J. Assoc. Public Anal.
J. Biochem. (Tokyo)
J. Biol. Chem.
J. Carbohydr. Chem.
J. Catal.
J. Chem. Educ.
J. Chem. Eng. Data
J. Chem. Inf. Comput. Sci.
J. Chem. Phys.
J. Chem. Res. (M)
J. Chem. Res. (S)
J. Chem. Soc., Chem. Commun.
J. Chem. Soc., Dalton Trans.
J. Chem. Soc., Faraday Trans. 1
J. Chem. Soc., Faraday Trans. 2
J. Chem. Soc., Perkin Trans. 1
J. Chem. Soc., Perkin Trans. 2
J. Chem. Thermodyn.
J. Chim. Phys. Phys.-Chim. Biol.
J. Chin. Chem. Soc. (Taipei)
J. Chromatogr.
J. Chromatogr. Sci.
J. Colloid Interface Sci.
J. Coord. Chem.
J. Cryst. Mol. Struct.
J. Doc.
J. Electroanal. Chem. Interfacial Electrochem.
J. Electrochem. Soc.
J. Electrochem. Soc. India
J. Fac. Sci. Univ. Tokyo
J. Fluorine Chem.
J. Food Sci.
J. Franklin Inst.
J. Gen. Chem. USSR (Engl. Transl.)
J. Hazard. Mater.
J. Heterocycl. Chem.
J. Histochem. Cytochem.
J. Indian Chem. Soc.
J. Indian Inst. Sci.
J. Inorg. Chem. USSR (Engl. Transl.)
J. Inst. Brew.
J. Inst. Chem. (India)
J. Inst. Fuel
J. Labelled Compd. Radiopharm.
J. Less-Common Met.
J. Lipid Res.
J. Liq. Chromatogr.
J. Lumin.
J. Macromol. Sci., Chem.
J. Macromol. Sci., Phys.
J. Magn. Reson.
J. Med. Chem.
J. Mol. Biol.
J. Mol. Catal.
J. Mol. Spectrosc.
J. Mol. Struct.
J. Neurochem.
J. Nonmet. Semiconduct.
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. Mashinostr.
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.
Liebigs 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
Mol. Cell. Biochem.
Mol. Cryst. Liq. Cryst.
Mol. Phys.
Monatsh. Chem.

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

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

Paint Manuf.
Pak. J. Sci.
Pak. J. Sci. Ind. Res.
Pak J. Sci. Res.
Periodia Polytech., Chem. Eng.
Pestic. Sci.
Philos. Mag.
Philos. Trans. R. Soc. London, A
Phosphorus Sulfur
Photochem. Photobiol.
Phys. Chem. Glasses
Phys. Rev.
Phys. Rev. Lett.
Phys. Scr.
Phytochemistry
Pigm. Resin Technol.
Pis'ma Zh. Eksp. Teor. Fiz.
Plast. Polym.
Pol. J. Chem.
Polyhedron
Polym. Age
Polym. Commun.
Polymer
Polym. Sci. USSR (Engl. Transl.)
Postepy Biochem.
Prikl. Biokhim. Mikrobiol.
Priroda (Moscow)
Proc. Am. Soc. Brew. Chem.
Process Biochem.
Processing
Proc. Indian Acad. Sci., Sect. A
Proc. Indian Acad. Sci., Sect. B
Proc., K. Ned. Akad. Wet., Ser. B
Proc., K. Ned. Akad. Wet., Ser. C
Proc. Natl. Acad. Sci., India, Sect. A
Proc. Natl. Acad. Sci. USA
Proc. R. Soc. Edinburgh, Sect. A
Proc. R. Soc. London, A
Proc. R. Soc. London, B
Proc. Soc. Exp. Biol. Med.
Prog. Bioorg. Chem.
Prog. Colloid Polym. Sci.
Prog. Inorg. Chem.
Prog. Med. Chem.
Prog. Nucleic Acid Res. Mol. Biol.
Prog. Nucl. Magn. Reson. Spectrosc.
Prog. Phys. Org. Chem.
Prog. React. Kinet.
Prog. Solid State Chem.
Prog. Stereochem.
Prog. Surf. Membr. Sci.
Prog. Surf. Sci.
Prog. Thin-Layer Chromatogr. Relat. Methods
Przem. Chem.
Pure Appl. Chem.
Pyrethrum Post

Quad. Ing. Chim. Ital.
Quim. Nova

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

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

Taehan Hwahakhoe Chi
Talanta
Technol. Rep. Osaka Univ.
Teor. Eksp. Khim.
Teor. Osn. Khim. Tekhnol.
Tetrahedron
Tetrahedron Lett.
Text. Res. J.
Theor. Exp. Chem. (Engl. Transl.)
Thermochim. Acta
Tin Its Uses
Top. Curr. Chem.
Top. Stereochem.
Trans. Inst. Met. Finish.
Transition Met. Chem. (Weinheim, Ger.)
Trant. J. Br. Ceram. Soc.
Trends Anal. Chem.
Trends Biochem. Sci.
Tr. Inst. Elektrokhim., Ural. Nauchn. Tsentr. Akad. Nauk SSSR

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

Vestn. Leningr. Univ., Fiz., Khim.
Vestn. Mosk. Univ., Ser. 2: Khim.
Vestn. Slov. Kem. Drus.
Vestsi Akad. Navuk BSSR. Ser. Khim. Navuk
Veszpremi Vegyip, Egy. Kozl.
Vitam. Horm. (N.Y.)
Vopr. Med. Khim.
Vysokomol. Soedin., Ser. A
Vysokomol. Soedin., Ser. B

Xenobiotica

Yakugaku Zasshi
Yuki Gosei Kagaku Kyokaishi

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

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.* 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[1,2]); 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 Internationale d'Unités' (SI). A detailed treatment is given in the so-called Green Book: *Quantities, Units and Symbols in Physical Chemistry* (Blackwell Scientific Publications, Oxford, 1993 edn.).

Guidelines for the publications of the Society. 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.

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*

Table 1 Base-units

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

Table 2 Prefixes

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

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^{-19} J
mass	unified atomic mass unit	u	u = 1.66041×10^{-27} kg

(8) *Other units now exactly defined in terms of the SI units.* These units are not part of the SI. It is recognized that their use may be continued for some time but it is recommended that except in special circumstances they should be progressively abandoned in conformity with international recommendations. The list given in Table 6 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. xxiii):

(*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.

Table 3 Derived units with special names and symbols

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

Table 4 Derived units with no special names or symbols

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

Table 5 Fractions and multiples of units with special names

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

Table 6 Units defined in terms of SI units

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

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

Specimen first page

Molecular Structures of the Gaseous Dimeric Molecules $Me_2Ga(\mu\text{-}H)_2GaMe_2$ and $Me_2Ga(\mu\text{-}Cl)_2GaMe_2$ as determined by Electron Diffraction

Paul L. Baxter,[a] Anthony J. Downs,*[,a] Michael J. Goode,[a] David W. H. Rankin*[,b] and Heather E. Robertson[b]

[a] *Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QR, UK*
[b] *Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, UK*

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, $Me_2Ga(\mu\text{-}X)_2GaMe_2$ (where X = H or Cl), with heavy-atom skeletons conforming to D_{2h} symmetry. Salient structural parameters in the r_a structures are: (*i*) for $[Me_2GaH]_2$, r(Ga · · · Ga) 261.0 (0.5), r(Ga–C) 195.4 (0.4) and r(Ga–H_b) 170.8 (1.4) pm; Ga–H_b–Ga 99.6 (1.4) and C–Ga–C 123.2 (1.5)°; (*ii*) for $[Me_2GaCl]_2$, r(Ga···Ga) 332.8 (1.9), r(Ga–C) 194.8 (0.3) and r(Ga–Cl_b) 238.2 (0.4) pm; Ga–Cl_b–Ga 88.6 (0.9) and C–Ga–C 135.4 (2.7)° ('b' denotes a bridging atom). Dimethylgallane thus represents the first gallium hydride containing a $Ga(\mu\text{-}H)_2Ga$ bridging unit to be characterised structurally; it is notable for the shortness of the Ga···Ga distance. The two molecules invite structural comparisons with related systems like $[Me_2EH]_2$ (E = B or Al), $[Me_2AlCl]_2$ and Ga_2Cl_6.

(*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.

(*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.

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 sructure 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 (μ).

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, β = 91.03(3)°, U = 4480 Å^3 (by least-squares refinement on diffractometer angles for 15 automatically centred reflections, λ = 0.710 69 Å), space group $P2_1/n$ (alt. $P2_1/c$, no. 14), Z = 4, D_c = 1.76 g cm^{-3}, $F(000)$ = 2160. Dark blue, air-sensitive tablets. Crystal dimensions (distance to faces from centre): 0.313(211,$\bar{2}\bar{1}\bar{1}$) × 0.163(010,$0\bar{1}0$) × 0.063(101,$\bar{1}0\bar{1}$) mm, μ(Mo-Kα) = 85.12 cm^{-1}.

Data Collection and Processing.[12]—CAD4 diffractometer, ω–2θ mode with ω scan width = 0.85 + 0.35 tan θ, ω scan speed 1.3–6.8° min^{-1}, graphite-monochromated Mo-Kα radiation; 6383 reflections measured ($1.5 \leqslant \theta \leqslant 25°$, $+h,k,l$), 5797 unique [merging R = 0.024 after absorption correction (max., min. transmission factors = 0.37, 0.10)], giving 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_{iso} [= 0.08(2) Å^2]. The weighting scheme $w = 1/[\sigma^2(F_o) + 0.0078F_o^2]$, with $\sigma(F_o)$ from counting statistics[12] gave satisfactory agreement analyses. Final R and R' 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: $C(2^{I}) \cdots C(2^{IV})$. 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 $Å^2$ or pm^2).

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

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

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 (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

---

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

and selected molecular dimensions contained within figure captions. The full data will be deposited at the Cambridge Crystallographic Data Centre. The inclusion of 'Series or Part numbers' in the title of Communications is not permitted. 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/updating 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.

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

Solution composition	
$[T_L]$ range/mol dm^{-3}	0.003–0.005
$[T_M]$ range/mol dm^{-3}	0.001–0.004
I/mol dm^{-3}, electrolyte	0.010, KNO_3
pH Range	2.7–10.8 (protonation)
Experimental method	pH Titration, calibrated in concentrations
T/°C	25
Total number of data points	
Protonation	207 (2 titrations)
Copper complexation	274 (3 titrations)
Method of calculation	SUPERQUAD $^{\text{reference}}$
Protonation constants (ligand = H_3L, errors as σ)	
$\log \beta_{HL}$	10.16 ± 0.01
$\log \beta_{H_2L}$	19.96 ± 0.01
$\log \beta_{H_3L}$	27.50 ± 0.02
$\log \beta_{H_4L}$	30.52 ± 0.03
Stability constants	
$\log \beta_{CuL}$	10.29 ± 0.09
$\log \beta_{CuHL}$	19.70 ± 0.01
$\log \beta_{CuH_2L}$	24.36 ± 0.05
$\log \beta_{Cu_2L_2}$	24.00 ± 0.05
$\log \beta_{Cu_2H_2L_2}$	3.66 ± 0.02

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.
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 β_{HL} *etc.*) and stability constants (log β_{CuHL}, log β_{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 *(conventional chemical structural diagram)*

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

a(Å) *with estimated error*		b(Å) *with estimated error*		c(Å) *with estimated error*	
alpha(deg.)*with estimated error*		beta(deg.) *with estimated error*		gamma(deg.) *with estimated error*	
Space Group	Z	R-factor(s) R wR	Temp(K)	Radiation ☐ X ☐ N	Powder Data Yes No ☐ ☐
Intensity Measurement ☐ densit. ☐ diffr. ☐ other(*specify*)			Volume(Å^3)	Mol. Weight	Mp(°C)
Absolute Configuration Determined ☐ Yes ☐ No		Colour CAS RN		Dm (g cm^{-3}) Dx (g cm^{-3})	

Polymorph Indicator *(eg. low-temp. form)*

Drug *(indicate, where appropriate, type of drug, activity, etc.)*

Disorder *(specify nature of disorder with reference to atom labels in coordinate list)*