# APPENDIX

## *IUPAC Publications on Nomenclature and Symbolism*

### 1.0 Compilations

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

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

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

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

1.3 Biochemical Nomenclature and Related Documents, a 220-page softcover manual published in 1978 by The Biochemical Society for IUB, and available from the Biochemical Society Book Depot, PO Box 32, Commerce Way, Colchester, Essex CO2 8HP. The contents are as follows:

*General*
Nomenclature of organic chemistry. Section E: Stereochemistry (1974)
Nomenclature of organic chemistry. Section F: Natural products and related compounds (1976)
Nomenclature of organic chemistry. Section H: Isotopically modified compounds (1977)
Isotopically labelled compounds: common biochemical practice
Recommendations for measurement and presentation of biochemical equilibrium data (1976)
Abbreviations and symbols for chemical names of special interest in biological chemistry (1965)
Abbreviations and symbols: a compilation (1976)
Citation of bibliographic references in biochemical journals (1971)
*Amino acids, peptides and proteins*
Nomenclature of α-amino acids (1974)
Symbols for amino-acid derivatives and peptides (1971)
Rules for naming synthetic modifications of natural peptides (1966)
Abbreviated nomenclature of synthetic polypeptides or polymerized amino acids (1971)
A one-letter notation for amino-acid sequences (1968)
Abbreviations and symbols for the description of the conformation of polypeptide chains (1969)
Nomenclature of peptide hormones (1974)
Recommendations for the nomenclature of human immunoglobulins
Protein data bank. A computer-based archival file for macromolecular structures (1977)
Nomenclature of multiple forms of enzymes (1976)
*Nucleotides and nucleic acids*
Abbreviations and symbols for nucleic acids, polynucleotides and their constituents (1970)
*Lipids*
Nomenclature of lipids (1976)

Nomenclature of steroids (1967)
Nomenclature of quinones with isoprenoid side chains (1973)
Tentative rules for the nomenclature of carotenoids (1970). Amendments (1974)
Nomenclature of tocopherols and related compounds (1973)
*Carbohydrates, etc.*
Tentative rules for carbohydrate nomenclature. Part 1 (1969)
Nomenclature of cyclitols (1973)
*Phosphorus-containing compounds*
Nomenclature of phosphorus-containing compounds of biochemical importance (1976)
*Miscellaneous*
Trivial names of miscellaneous compounds of importance in biochemistry (1965)
Nomenclature and symbols for folic acids and related compounds (1965)
Nomenclature for vitamins B-6 and related compounds (1973)
Nomenclature of corrinoids (1973)

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

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

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

1.6 Quantities, Units, and Symbols in Physical Chemistry, a 134-page hardcover volume published in 1988, available from Blackwell Scientific Publications, Oxford.

## 2.0 Documents not included in the compilations

### 2.1 Nomenclature of Elements and Compounds

2.1.1 *Amino acids and Peptides*

Nomenclature and symbolism for amino acids and peptides (*Pure Appl. Chem.*, 1984, **56**, 595; *Eur. J. Biochem.*, 1984, **138**, 9).

2.1.2 *Analytical Reagents*

Guide to trivial names, trade names, and synonyms for substances used in analytical chemistry (*Pure Appl. Chem.*, 1978, **50**, 339).

2.1.3 *Boron Compounds*

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

2.1.4 *Carbohydrates*

Conformational nomenclature for five- and six-membered ring forms of monosaccharides and their derivatives (provisional) (*Pure Appl. Chem.*, 1981, **53**, 1901; *Eur. J. Biochem.*, 1980, **111**, 295).

Abbreviated terminology of oligosaccharide chains (provisional) (*Pure Appl. Chem.*, 1982, **54**, 1517; *J. Biol. Chem.*, 1982, **257**, 2347).

Polysaccharide nomenclature (provisional) (*Pure Appl. Chem.*, 1982, **54**, 1523; *J. Biol. Chem.*, 1982, **257**, 3352).

Nomenclature of unsaturated monosaccharides (provisional) (*Pure Appl. Chem.*, 1982, **54**, 207; *Eur. J. Biochem.*, 1981, **119**, 1; errata *Eur. J. Biochem.*, 1982, **125**, 1).

Nomenclature of branched-chain monosaccharides (provisional) (*Pure Appl. Chem.*, 1982, **54**, 211; *Eur. J. Biochem.*, 1981, **119**, 5; errata *Eur. J. Biochem.*, 1982, **125**, 1).

Symbols for specifying the conformation of polysaccharide chains (provisional) (*Pure Appl. Chem.*, 1983, **55**, 1269; *Eur. J. Biochem.*, 1983, **131**, 5).

2.1.5 *Delta Convention*

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

2.1.6 *Elements*

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

2.1.7 *Enzymes*

Enzyme Nomenclature (1984), published by Academic Press in hardcover and softcover editions.

2.1.8 *Folic Acid*

Nomenclature and symbols for folic acid and related compounds (*Pure Appl. Chem.*, 1987, **59**, 833; *Eur. J. Biochem.*, 1987, **168**, 251).

2.1.9 *Glycoproteins*

Nomenclature of glycoproteins, glycopeptides, and peptidoglycans (*Pure Appl. Chem.*, 1988, **60**, 1389).

2.1.10 *Heterocyclic Compounds*

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

2.1.11 *Hydrogen*

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

2.1.12 *Isotopically Modified Compounds*

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

2.1.13 *Lambda Convention*

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

2.1.14 *Nitrogen Hydrides*

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

2.1.15 *Nucleotides*

Abbreviations and symbols for the description of conformations of polynucleotide chains (provisional) (*Pure Appl. Chem.*, 1983, **55**, 1279; *Eur. J. Biochem.*, 1983, **131**, 9).

2.1.16 *Numerical Terms*

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

2.1.17 *Polymers*

Nomenclature of regular single-strand organic polymers (*Pure Appl. Chem.*, 1976, **48**, 373).

Nomenclature for regular single-strand and quasi single-strand inorganic and co-ordination polymers (*Pure Appl. Chem.*, 1985, **57**, 149).

Source-based nomenclature for copolymers (*Pure Appl. Chem.*, 1985, **57**, 1427).

Stereochemical definitions and notations relating to polymers (*Pure Appl. Chem.*, 1981, **53**, 733).

Use of abbreviations for names of polymeric substances (*Pure Appl. Chem.*, 1987, **59**, 691).

Basic definitions of terms relating to polymers (*Pure Appl. Chem.*, 1974, **40**, 477).

Definitions of terms relating to individual macromolecules, their assemblies, and dilute polymer solutions (*Pure Appl. Chem.*, 1989, **61**, 211).

A classification of linear single-strand polymers (*Pure Appl. Chem.*, 1989, **61**, 243).

Definition of terms relating to crystalline polymers (*Pure Appl. Chem.*, 1989, **61**, 769).

2.1.18 *Polyanions*

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

2.1.19 *Prenols*

Nomenclature of prenols (*Pure Appl. Chem.*, 1987, **59**, 683; *Eur. J. Biochem.*, 1987, **167**, 181).

2.1.20 *Retinoids*

Nomenclature of retinoids (provisional) (*Pure Appl. Chem.*, 1983, **55**, 721; *Eur. J. Biochem.*, 1982, **129**, 1).

2.1.21 *Steroids*

Nomenclature of steroids (*Pure Appl. Chem.*, 1989, **61**, 1783).

2.1.22 *Tetrapyrroles*

Nomenclature of tetrapyrroles (*Pure Appl. Chem.*, 1987, **59**, 779).

2.1.23 *Tocopherols*

Nomenclature of tocopherols and related compounds (*Pure Appl. Chem.*, 1982, **54**, 1507; *Eur. J. Biochem.*, 1982, **123**, 473).

2.1.24 *Vitamins*

Nomenclature of Vitamin D (provisional) (*Pure Appl. Chem.*, 1982, **54**, 1511; *Eur. J. Biochem.*, 1982, **124**, 223).

2.1.25 *Zeolites*

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

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

2.2.1 *General*

Glossary of terms used in physical organic chemistry (*Pure Appl. Chem.*, 1983, **55**, 1281).

2.2.2 *Analytical*

Nomenclature, symbols, units, and their usage in spectrochemical analysis. Part VII, Molecular absorption spectroscopy, UV and visible (*Pure Appl. Chem.*, 1988, **60**, 1449). Part X, Preparation of materials for analytical atomic spectroscopy (*Pure Appl. Chem.*, 1988, **60**, 1461).

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

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

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

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

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

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

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

2.2.3 *Clinical*

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

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

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

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

2.2.4 *Colloids and Surface Chemistry*

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

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

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

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

2.2.5 *Electrochemistry*

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

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

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

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

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

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

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

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

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

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

2.2.6 *Kinetics*

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

2.2.7 *Photochemistry*

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

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

2.2.8 *Quantum Chemistry*

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

2.2.9 *Reactions*

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

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

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

2.2.10 *Rheological Properties*

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

2.2.11 *Spectroscopy*

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

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

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

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

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

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

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

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

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

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

2.2.12 *Thermodynamics*

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

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

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

# JOURNALS OF THE ROYAL SOCIETY OF CHEMISTRY

# Refereeing Procedure and Policy (1991)

## 1.0 Contributions to Dalton, Perkin and Faraday Transactions, J. Mater. Chem., The Analyst, J. Anal. At. Spectrom. and J. Chem. Research

### 1.1 Introduction

This document summarises the procedure used for assessing papers submitted to the four *Transactions, J. Mater. Chem., The Analyst, J. Anal. At. Spectrom.*, and *J. Chem. Research*, and provides guidelines for referees engaged in this assessment.

### 1.2 Subject matter

Papers are submitted to the various journals according to subject matter. If it is felt that a paper would be published more appropriately in an RSC journal other than the one suggested by the author, the referee should inform the Editor. The topics covered by the various journals are as follows.

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

*Faraday Transactions* (*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.

*Journal of Materials Chemistry*. The chemistry of materials, particularly those associated with advanced technology; modelling of materials; synthesis and structural characterisation; physicochemical aspects of fabrication; chemical, structural, electrical, magnetic and optical properties; applications.

*The Analyst* (*Analytical Chemistry*). Theory and practice of all aspects of analytical chemistry, fundamental and applied, inorganic and organic, including chemical, physical, and biological methods.

*Journal of Analytical Atomic Spectrometry*. The development and analytical application of atomic spectrometric techniques.

*Journal of Chemical Research*. All areas of chemistry. The format of this journal (one- or two-page printed synopsis in Part S, plus microform version of authors' full text typescript in Part M) makes it particularly suitable for papers containing lengthy experimental sections or extensive data tabulations.

### 1.3 Procedure

Each manuscript is considered independently by two referees. The referees' reports constitute recommendations to the appropriate Editorial Board, which is empowered to take final action on manuscripts submitted. The Editor, acting for the Editorial Board, is responsible for all administrative and executive actions, and is empowered to accept or reject papers. It is the Editor's duty to see that, as far as possible, agreement is reached between authors and referees; although the referees may need to be consulted again concerning an author's reply to comments, further refereeing will be avoided as far as possible.

1.3.1 *Adjudication of disagreements.* If there is a notable discrepancy between the reports of the two referees, or if the difference between authors and referees cannot be resolved readily, a third referee may be appointed as adjudicator. In extreme cases, differences may be reported to the appropriate Editorial Board for resolution.

When a paper is recommended for rejection by referees, the Editor will inform the authors and return 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. The Editor may refer to the Editorial Boards any papers which have been recommended for acceptance by the referees, but about which the Editor is doubtful.

1.3.2 *Anonymity.* The anonymity of referees is strictly preserved, and reports should be couched in terms which do not disclose the identity of the writer. A referee should never communicate directly with an author, unless and until such action has been sanctioned by the Society, through the Editor.

1.3.3 *Confidentiality.* A referee should treat a paper received for assessment as confidential material. Information acquired

by a referee from such a paper is not available for citation until the paper is published.

## 1.4 Policy

The primary criterion for acceptance of a contribution for publication is that it should advance scientific knowledge significantly. Papers that do **not** contain new experimental results may be considered for publication **only** if they either reinterpret or summarise known facts or results in a manner presenting an advance in chemical knowledge. Papers in interdisciplinary areas are acceptable if the chemical content is considered satisfactory.

Papers reporting results regarded as **routine** or **trivial** are not acceptable in the absence of other, desirable attributes.

Although short papers are acceptable, the Society strongly discourages the **fragmentation** of a substantial body of work into a number of short publications; such fragmentation is likely to be grounds for rejection.

The **length** of an article should be commensurate with its scientific content; however, authors are allowed every latitude (consistent with reasonable brevity) in the **form** in which their work is presented. Figures and flow-charts can often save space as well as clarify complicated arguments, and should not be excised unless they are unhelpful or really extravagant.

If a paper as a whole is judged suitable for the *Journal*, minor criticisms should not be unduly emphasised. It is the responsibility of the Editor to ensure the use of reasonably brief phraseology, and to assist the author to present his work in the most appropriate format.

However, referees should not hesitate to recommend rejection of papers which appear incurably badly composed.

It should be clearly understood that referees' reports are made in confidence to the Editor, at whose discretion comments will be transmitted to the author. To assist the Editor, referees are requested to indicate which comments are designed only for consideration, as distinct from those which, in the referee's view, require specific action or an adequate answer before the paper is accepted.

Referees may ask for sight of **supporting data** not submitted for publication, or for sight of a previous paper which has been submitted but not yet published. Such requests must be made to the Editor, not directly to the author.

1.4.1 *Authentication of new compounds.* Referees are asked to 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 the Society's policy is that evidence for the unequivocal identification of new compounds should wherever possible include good elemental analytical data; for example, 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.

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.

Referees are reminded of the need to be exacting in their standards but at the same time flexible in their admission of evidence. It remains the Society's policy to accept work only of high quality and to permit no lowering of standards.

## 1.5 Titles and summaries

Referees should comment on titles and summaries with the following points in mind.

Titles of papers are used out of context by several organisations for current awareness purposes. To enable such systems to serve chemists adequately, titles must be written around a sufficient number of scientific words carefully chosen to cover the important aspects of the paper.

Summaries should preferably be self-contained, so that they can be understood without reference to the main text.

## 1.6 Speed of Refereeing

The Editorial Boards are anxious to maintain and to reduce further if possible the publication times now being achieved. In this connection, referees should submit their reports with the minimum of delay, or return manuscripts immediately to the Editor if long delay seems inevitable.

## 1.7 Suggestion of Alternative Referees

The Editor welcomes suggestions of alternative referees competent to deal with particular subject areas. Such suggestions are particularly helpful in cases where referees consider themselves ill-equipped (in terms of specialist knowledge) to deal with a specific paper, and in highly specialized or new areas of research where only a limited number of experts may be available. If, in such a case, the alternative and the original referee work in the same institution, the manuscript may be passed on directly after informing the Editor.

## 1.8 Notes (Short Papers) and Letters

'Notes' are published in *Dalton Transactions*; the corresponding format in *The Analyst* and *J. Anal. At. Spectrom.* is referred to as a 'short paper'. These articles are intended for the description of essentially complete pieces of work which are not of the length to justify a full paper. They are *NOT* preliminary communications, nor in any way an alternative to *Chemical Communications*, for which there are additional criteria of novelty and urgency. The quality of material contained in a note (short paper) should be the same as that in a full paper. Investigations arising out of some larger project but not prosecuted to the same degree are particularly appropriate for this format.

A note (short paper) should not normally exceed in length about 8 pages of typescript, including figures, tables, *etc.* It should comprise a short abstract (except in *The Analyst* and *J. Anal. At. Spectrom.*) and discussion, but adequate experimental details are required.

In *J. Chem. Research*, a 'short paper' is essentially of the same type. As a consequence of its length, it appears in full in Part S with no microform version in Part M.

'Letters', published only in *Dalton Transactions*, are a medium for the expression of scientific opinions and views normally concerning material published in that journal; it is intended that contributions in this format should be published rapidly. The letters section is for scientific discussion, and is 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 consideration for publication alongside the original letter.

### 1.9 Relationship with Communications Journals

In cases where a preliminary report of the work described has appeared (for example in *Chemical Communications*), referees should alert the editor to any excessive and unnecessary repetition of material; this can arise in connection with communications journals in which the restrictions on length and the reporting of experimental data are less severe than those of *Chemical Communications*. Furthermore, the acceptability of the full paper must be judged on the basis of the significance of the additional information provided, as well as on the criteria outlined in the foregoing sections.

## 2.0 Contributions to Chemical Communications

*Chemical Communications* 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 in most cases by full papers in other journals, providing detailed accounts of the work. It is Society policy that only a fraction of research work warrants publication in *Chemical Communications*, and strict refereeing standards should be applied. The benefit to the reader from the rapid publication of a particular piece of work before it appears as a full paper must be balanced against the desirability of avoiding duplicate publication. The needs of the reader, not the author, must be considered, and priority in publication should not be allowed to determine acceptability. Acceptance should be recommended only if, in the opinion of the referee, the content of the paper is of such urgency that rapid publication will be advantageous to the progress of chemical research.

The length of Communications is strictly limited; only in exceptional circumstances should it exceed one printed page (two-and-a-half to three A4 pages of typescript) and referees should be particularly critical of manuscripts longer than this. Communications do not contain extensive spectroscopic or other experimental data, but referees may ask for sight of such data before reaching a decision.

The refereeing procedure for Communications is the same as that for full papers, except that rapidity of reporting is crucial in order to maintain rapid publication. The Journals Committee functions as the Editorial Board of *Chemical Communications* and as such acts as final arbiter in cases of dispute.

## 3.0 Communications submitted to The Analyst and J. Anal. At. Spectrom.

Criteria for acceptance of communications submitted to *The Analyst* and *J. Anal. At. Spectrom.* are similar to those for contributions to *Chemical Communications*, except that they should be concerned specifically with analytical chemistry. However communications to *The Analyst* and *J. Anal. At. Spectrom.* are not subjected to refereeing in the usual way; a decision whether or not to publish rests with the Editor, who may or may not obtain advice from a referee.

## 4.0 Communications submitted to Perkin or Faraday Transactions or J. Mater. Chem.

Criteria for acceptance of Communications submitted to *Perkin* or *Faraday Transactions* or *J. Mater. Chem.* are similar to those for contributions to *Chemical Communications*, except that the work will be of more specialist interest. For *Perkin Communications* inclusion of key experimental data is expected. Assessment is carried out by a small nucleus of referees, consisting largely of members of Perkin Editorial Board or of the Faraday or Materials International Advisory Editorial Board, as appropriate.

## 5.0 Contributions to Mendeleev Communications

*Mendeleev Communications*, published jointly by the Royal Society of Chemistry and the USSR Academy of Sciences, is a sister publication to *Chemical Communications*, containing preliminary reports of the same type, in any area of chemistry. The majority of contributions are from Soviet authors.

Assessment involves two stages of refereeing. Manuscripts submitted to the Soviet Editorial Office are refereed initially by a Soviet scientist. If found acceptable they are then reviewed by Western scientists chosen by the Royal Society of Chemistry. A favourable recommendation at this stage, from one referee, is sufficient authority for acceptance. If the recommendation is unfavourable, however, a second RSC referee is consulted; two unfavourable reports are required for rejection. Manuscripts submitted to the UK Editorial Office undergo this two-stage refereeing process in reverse.

## 6.0 X-Ray Crystallographic Work

6.1 Crystallographic papers are of two types:

(A) The majority, which contain definitive data on completely refined determinations.

(B) A minority which include brief accounts of structures containing feature(s) of unusual interest and where the structure solutions are clear but where (for any of a variety of reasons) the full refinement has not been completed. These are then regarded as preliminary publications, at least so far as the X-ray results are concerned.

Both types of publication are appropriate for *Chem. Commun.*; only those of type (A) should normally appear in *Dalton* or *Perkin Transactions*.

6.2 Papers of type (A) in *Dalton* and *Perkin Transactions* should normally contain the information in their *titles* that an X-ray structure determination has been carried out; this is often appropriate in *Chem. Commun.* also, but not obligatory. Papers of type (B) need not do so if the X-ray determination forms only a minor part. *Summaries* should always contain this information unless the paper is of type (B) and the structure determination is not a main point of the communication.

6.3 All papers containing crystallographic determinations will be refereed by two referees, one a structural chemist. If the editor considers it advisable, the paper may also be sent to a crystallographer for comment. Referees will not normally be expected to check values of structural parameters for publication (*e.g.* bond lengths and angles against atomic co-ordinates; this will be done after publication by CCDC or Bonn), but should still pay attention to the quality of the experimental crystallographic work. However their primary concern should be such new chemistry as is involved in the structure.

6.4 On occasions *Chem. Commun.* will publish preliminary accounts [type (B)] of crystal structures of unusual *chemical* interest. By 'preliminary' is meant that the data have not yet been fully refined. Sufficient supplementary data must be provided for the referee to judge whether the 'not-fully-refined' structure does indeed prove the desired point, and care should be taken by the referees to ensure that the authors do not overstate the case they have—for example by reporting bond

lengths to very high degrees of apparent precision when they have poor *R*-factors. Such papers will always be refereed by a professional crystallographer. Authors must indicate in the paper or the supplementary data the justification for publishing without full refinement and referees should comment on whether the case for publication is convincing.

6.5 In many cases the structure referred to in *Chem. Commun.* will be fully refined. The *Chem. Commun.* can then be considered to fulfil the archival function, and the structure determination may not require further detailed refereeing when presented as part of a full paper. In the full paper, the author's purpose will then be served by a simple reference back to the original communication. However, if the crystallography is discussed again at any length in the full paper, the data should be re-presented to the referees in full, and re-published if considered necessary.

6.6 There may be other cases when an author wishes to publish a paper in *Dalton* or *Perkin* in which the result of a crystal structure determination is discussed, but in which details or extensive discussion are considered unnecessary. The crystallographer may even be omitted as a co-author (for example when the determination is carried out by a commercial company). If the author is able to show the referees that this procedure is appropriate, it will be allowed provided that it does not lead to unnecessary fragmentation. However, the author must provide, as supplementary information, sufficient data relating to the crystal structure determination to allow a referee to make sure that the point made is correct, and co-ordinates *etc.* will be deposited with CCDC (or Bonn). The brief published description of the determination should be supplemented by appropriate reference to 'unpublished work'.

**CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE**

**ABSTRACT FORM**

| Contributor (name and address) |
|---|
| |

| Compound Name |
|---|
| |

| Synonym |
|---|
| |

| Authors |
|---|
| |

| Journal Reference (name or coden, volume, page, year) |
|---|
| |

Cell Dimensions with Standard Deviations

| a(Å) | b(Å) | c(Å) |
|---|---|---|
| alpha | beta | gamma |

| Volume | Mol.Weight | Dm | Dx | Z | Space Group |
|---|---|---|---|---|---|
| | | | | | |

| Corrected Bond Lengths in Paper | Temp(°K) | Mp(°C) | Powder Data | Radiation |
|---|---|---|---|---|
| ☐ Yes ☐ No | | | ☐ Yes ☐ No | ☐ X ☐ N |

| Intensity Measurement | No. of Reflections | No. of Parameters | R-factor |
|---|---|---|---|
| ☐ densit. ☐ diffr. ☐ other | | | |

| Absolute Configuration | Colour | Polymorph Indicator | CAS Registry Number |
|---|---|---|---|
| ☐ Yes ☐ No | | | |

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

Chemical Classification (to be assigned by CCDC staff)

Formula (each residue to be formulated separately)

Diagram (conventional chemical structural diagram)

Disorder (specify nature of disorder with reference to atom labels in coord. list)

Remarks (details of constrained refinement, publication history, etc.)