HELVETICA CHIMICA ACTA

Instructions to Authors (1996)

1. General Policy

The journal *Helvetica Chimica Acta* (*HCA*) is published by the New Swiss Chemical Society (NSCS). Contributions from all fields of pure chemistry may be submitted.

HCA publishes original articles, preliminary communications, and notes. Review articles will not be accepted for publication in *HCA*.

Contents of manuscripts submitted to *HCA* should not have been published previously, except in the form of a brief preliminary communication, nor submitted to another journal. The decision to accept a contribution rests with the Editorial Board of the *HCA*.

2. Forwarding Address

Manuscripts should be submitted in *triplicate* together with a transmittal letter signed by the author to whom correspondence should be addressed to:

Helvetica Chimica Acta
Prof. Ch. Tamm
Postfach 313
CH–4010 Basel
Switzerland

Correspondence concerning submitted manuscripts should be mailed to the same address, quoting the manuscript reference number.

3. Copyright

Submission of a manuscript implies that the authors agree to transfer copyright to the NSCS when the contribution is accepted for publication. Reproduction of the text, figures, or tables from *HCA* is allowed only with permission of the Editorial Office.

4. Preparation of Manuscripts

4.1. *General Considerations.* Manuscripts may be submitted in German, French, Italian, or English. They must be typewritten, double-spaced, on substantial paper of A4 or similar format. Authors are requested to reserve margins of at least 3 cm at the top and bottom of each page and at least 4 cm on the left-hand side. Copies made by a clearly legible duplication process are preferred. Computer-processed manuscripts must be of typewriter quality.

Pages should be numbered consecutively beginning with the title page. References, tables, figure legends, formula collections, schemes, and figures *must* be grouped together

in this order at the end of the manuscript and numbered accordingly. Original drawings of formulae, schemes, and figures should be furnished together with the manuscript.

Manuscripts should be kept to minimum length. For clarity, they should be subdivided into labeled sections *e.g.* **Introduction, Results, Discussion, Experimental Part.**

Special types of print should be indicated as follows:

Specification of Typeface

Type	Mark	Symbol	Example	Example (printed)
Boldface[a])	Single underline		Introduction	**Introduction**
Italic[b])	Wave-like underline		in vitro	*in vitro*
Small capital[c])	Double underline		0.5M	0.5M
Boldface italic[d])	Underline with wavy line		R	***R***

[a]) Headings, designated numbers of chemical compounds.

[b]) Subheadings, configurational prefixes ((*R*)-, (*S*)-, *cis*-, *trans*-, *etc.*), Latin words or abbreviations, words in languages other than English, trade names of chemical compounds (first letter should be capitalized), names of authors if mentioned in the text.

[c]) Symbols of molar and normal concentrations (M and N), D- and L-, the names or initials of the nomenclature of genera, species, or varieties.

[d]) The italicized terms and prefixes in headings.

Special characters not available on a typewriter should be clearly indicated in ink and explained unambiguously in the margin on their first appearance.

4.2. *Title Page.* The lay-out of the title page should be modelled on the example shown on p. 3. A current issue of *HCA* should also be consulted.

Attention is drawn to the following points:

a) The title of a manuscript should reflect concisely the purpose and findings of the work in order to provide maximal information for a computerized title search. Abbreviations, symbols, chemical formulae, references, and footnotes should be avoided. First letters of nouns and adjectives are capitalized.

b) The authors' full first names, middle initials, and last names should be given, followed by the address (or addresses) of the contributing laboratory (laboratories). The author to whom correspondence and/or inquiries should be directed should be indicated by an asterisk (*). Footnotes may be added to indicate the present mailing address(es) of the author(s).

The complete address, *including phone number* (telefax number if any), of the correspondence author should also be given.

4.3. *Summary.* The second page of the manuscript should be reserved for a summary in English, independent of the language of the main text. If this is German, French, or Italian, the summary should be preceeded by an English translation of the title. ***The summary should be self-explanatory and intelligible without reference to the text and should not exceed 200 words for manuscripts in English.***

4.4. *References.* References should be numbered sequentially in the order they are cited in the text. The numbers should be set in brackets, thus [2] or [3] [14]. References typed with double spacing are to be collected in numerical order at the end of the main text. Titles of journals must be abbreviated according to *Chemical Abstracts* (*cf. Chemical Abstracts Service Source Index* (*CASSI*) and *Appendix I*), *e.g.*:

Prof. F. Gerson
Tel. (061) 321 46 55

ESR-Spectroscopical Investigation of Radical Ions
Part 23[1)]

Radical Ions of Conjugated Polycyclic Hydrocarbons Containing Two Phenalenyl π-Systems

by Fabian Gerson*, Jürgen Knöbel, and André Metzger[2)]
Institut für physikalische Chemie der Universität Basel,
Klingelbergstrasse 80, CH-4056 Basel

and Ichiro Murata and Kazuhiro Nakasuji
Department of Chemistry, Faculty of Science,
Osaka University, Toyonaka, Osaka 560, Japan

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1) Part 22: [1].

2) Present address: Ciba-Geigy SA, CH-4133 Schweizerhalle.

[1] M. Nakane, C.R. Hutchinson, H. Gollmann, *Tetrahedron Lett.* **1980,** *21,* 1213.
[2] R.J. Ferrier, P. Prasit, *J. Chem. Soc., Chem. Commun.* **1981,** 983; A.J. Kirby, R.J. Martin, *ibid.* **1979,** 1079.
[3] R.S. Davidson, in 'Molecular Association', Ed. R. Foster, Academic Press, New York, 1975, Vol. 1, pp. 215–334.
[4] Y.A. Ovchinnikov, 'Proceedings of the 36th International Meeting of the Société de Chimie Physique – Paris (September 82)', in 'Physical Chemistry of Transmembrane Ion Motion', Ed. G. Spach, Elsevier, Amsterdam, 1983, Vol. 24.

[5] J. F. Feeman, to *Crompton & Knowles Corp.*, U.S. Patent 3,098,096, 1983.
[6] F. Gerson (Institut für physikalische Chemie der Universität Basel, Klingelbergstrasse 80, CH–4056 Basel), personal communication.

Attention is drawn to the following conventions:

a) Names of all authors of cited publications should be given. Use of '*et al.*' in the list of references is not acceptable.

b) Only the initials of first and middle names should be given.

c) The name of the journal and volume number cited should be underscored with a wavy line (italics).

d) Whenever possible, composite references should be used, instead of a series of individual ones. The abbreviation '*ibid.*' may only be used within such a composite reference.

e) In references described as 'personal communications', an affiliation should follow the name(s) of the person(s).

In the text, reference to author(s) of cited works should be made without giving initials, *e.g.* '... as shown by *Jones* and *Smith* [7]'. If the reference carries the names of three or more authors it should be quoted as '... *Smith et al.* [3]', if *Smith* is the first author, or as '*Jones* and coworkers [3]', if *Jones* is the senior author.

4.5. *Footnotes.* Footnotes, *i.e.* explanations or comments on the text, should be kept to a minimum. They should be indicated in the manuscript by parenthesized superscripts, *e.g.* '... is implied[1]), otherwise ...', and numbered sequentially. Each footnote should be *typed double-spaced* at the bottom of the page of the manuscript in which it is first mentioned. Footnotes should not be included among the 'References'.

4.6. *Tables.* Tables should be used only in case they will present information more effectively than running text. Numbered tables with suitable captions at the top should be typed on separate sheets and placed after the references. Each table must be referred to in the text. Column headings should be as short as possible but must define units unambiguously. When necessary, an abbreviated or symbolic column heading should be used and explained in the table-heading or in a footnote. Footnotes to tables should be labeled [a]), [b]), [c]) *etc.*, and typed at the bottom of the table. Tables should be prepared to fit the page format of *HCA*.

4.7. *Structural Formulae, Schemes, and Figures.* Line drawings or sharp glossy photographs (no *Xerox* or similar copies) of the figures and structural formulae should be submitted with the manuscript. Copies must be included with each copy of the manuscript.

Original drawings of standard size A4 are preferred. In any case drawings should not exceed the standard size A3 (about 30 × 40 cm) and must contain all necessary symbols and lettering, *i.e.* they must be usable without additional art work by the *HCA* printers.

Line thickness, line spacings, and size of lettering should be planned for optimal reproduction (*cf. Appendix II*). Computer-plotted drawings must satisfy the same criteria.

Original drawings or photographs should be identified with the author's name and numbered to agree with the figure legends.

Structural formulae will not be type-set and must, therefore, be provided by the authors ready for reproduction. They should be combined in suitable schemes to reduce the cost of block-cutting. In general, only displayed formulae should be given key numbers; compounds mentioned only in the text should be referred to by name.

For authors using the *ChemDraw* program, the following preference items are recommended: fixed length, 25 pt; line width, 1 pt; bold width, 3 pt. Single-width bold and dashed lines are preferred to wedges for stereochemical notation; 14-pt *Helvetica* font should be used for text material, and 12-pt *Helvetica* font for atom labels. Drawings should be prepared with the page setup at 70% and printed in this manner with a laser printer on a good quality *white paper*. For an example of the desired appearance, see B. Maurer, A. Hauser, J.-C. Froidevaux, *Helv. Chim. Acta* **1989,** *72,* 1400.
Color reproduction in Figures and/or Formulae is possible. The Editorial Office will provide the authors with an estimate of charges which they have to bear.

4.8. *Chemical Equations and Physical or Mathematical Expressions.* Chemical equations and physical or mathematical expressions should be numbered sequentially on the right-hand side with arabic numerals in parentheses. Physical quantities and variables that have to be defined in the text should be written in *italics* (wavy line). It is recommended to use the symbols proposed by IUPAC (*cf. Pure Appl. Chem.* **1979,** *51,* 1).

Fractional expressions should be written using a slant, *e.g. hν/kT.*

5. Nomenclature

All new compounds should be named in accordance with IUPAC rules (*cf. Appendix III*). As an additional guideline the *Index Guide of Chemical Abstracts* should be consulted. Some special conventions peculiar to *HCA* are:

For common solvents, reagents, or other compounds, the molecular formulae or accepted abbreviations may be used: *e.g.* $CHCl_3$, NaCl, $SOCl_2$, MeOH, DMF, DMSO, THF, Py.

Different alkyl or arylalkyl radicals should be designated by superscripts: R^1, R^2, R^3 *etc.* (Subscripts denote the number of radicals.) Aryl radicals should be designated by Ar^1, Ar^2, *etc.*, all others by X, Y, *etc.* (*e.g.* X = O, Y = NH_2, Z = Br).

Individual atoms should be referred to as C(2), N(5) (not C-2 and N-5), *etc.* For 'hydrogen atom attached to carbon atom 4', *etc.*, *HCA* prefers the notation H–C(4).

An *ad hoc* abbreviation may be used for a name or formula that occurs repeatedly. This has to be clearly defined, *e.g.* THC = tetrahydrocannabinol.

Some symbols and abbreviations are listed in *Appendix IV.*

6. Units and Their Symbols

SI units are to be used, especially in contributions dealing with physical chemistry. However, some non-SI units listed in *Appendix V* are acceptable.

7. Special Instructions Concerning Contributions Containing X-Ray Crystal-Structure Results

All contributions which report the results of an X-ray crystal-structure determination, even in a minor way, must adhere to the following instructions.

While the results of crystal-structure determinations are of interest to readers of *HCA*, a detailed description of the experiment is usually not necessary. However, sufficient information must be provided to enable the referees to assess the quality of an X-ray structure determination, and for deposition in one of the crystallographic databases. The crystallographic information should be provided in *two* parts, the first to appear in the *printed paper* and the second as *supplementary material.* Unless the authors specifically wish to highlight particular aspects of the structure or the experiment, the minimum experimental information to be provided in each part is as follows:

1. *Printed Paper*

a) *Information to be contained within the* Discussion *Section:*

- A brief description of the structure where appropriate, or if unusual features are present
- A labelled view of the molecule ***with thermal ellipsoids, not arbitrary spheres***
- A table of important bond lengths, angles, or torsion angles, if appropriate
- Other tables and diagrams, if relevant to the discussion of the results

Full tables of refined atomic coordinates, bond lengths, and angles, and related information will only be printed if *specifically* requested by the authors, and if the Referees agree that the information is essential to the understanding of the discussion.

b) *Information which must be contained within the* Experimental Part:

A brief description of the procedures used for data collection, structure solution, and refinement. For routine analyses, this need not amount to more than a few sentences, but unusual parameters or procedures should be described. Crystallographic nomenclature and conventions should conform to the usage of *International Tables for Crystallography*. The following items should be given explicitly:

- Systematic name, *Chemical Abstracts* Reg. No., or other identifying name
- Source of material and solvent for crystallization
- Chemical formula
- Formula weight
- Unit cell dimensions and volume with standard uncertainties
- Crystal system and space group
- Number of molecules or formula units per unit cell
- Diffractometer used
- Radiation and wavelength
- Temperature and pressure of measurement (if different from 298 K and 1 atm)
- Calculated density D_x (and measured density, D_m, if applicable)
- Linear absorption coefficient
- Method of measuring intensities
- Max. value of $(\sin\theta)/\lambda$ or θ reached in intensity measurements
- Type of absorption correction applied (if applicable) and max. and min. values of correction
- Decay correction (if applicable) with maximum decay value
- Method used to solve and refine structure including treatment of H-atoms
- Use of F or F^2 magnitudes in least-squares refinement
- Number of measured, independent and observed reflections
- Criterion for classifying reflections as observed $[I > n\sigma(I)]$
- Number of parameters refined
- Final values of $R = \Sigma \| |F_o| - |F_c| \| / \Sigma |F_o|$, $wR = [\Sigma w(|F_o| - |F_c|)^2 / \Sigma w F_o^2]^{1/2}$ and $s = [\Sigma w(|F_o| - |F_c|)^2 / (N_o - N_v)]^{1/2}$ (or the F^2 equivalents)
- Max. positive and max. negative electron density in final *Fourier* synthesis.
- For polar structures, reason for choice of enantiomorph or method of testing absolute configuration
- All computer programs used

2. *Supplementary Material and Deposition of Crystallographic Data*

The supplementary material is required for refereeing purposes and for deposition in one of the crystallographic databases. The Editor will deposit the crystallographic data with the *Cambridge Crystallographic Data Centre* (*CCDC*) or in the *Inorganic Crystal Structure Database* (*ICSD*), as appropriate, when the printed paper appears.

Authors are encouraged to submit all supplementary crystallographic data using the *Crystallographic Information File* (*CIF*) format (see *Acta Crystallogr., Sect. A* **1991,** *47,* 655), but other formats will also be accepted. *CIF* files are readily produced with most current structure refinement packages and usually contain all of the information that is required. Supplementary material produced in this way can be deposited electronically, as described below.

To facilitate the deposition of data with the *CCDC*, the Centre has developed an electronic deposition form. This form can be combined with a *CIF* or tables of data that are in other formats.

The information required for deposition includes:

1) An electronic deposition form for each crystallographic determination. This form can be obtained from the *CCDC* in one of two ways:

– send an e-mail message to: **fileserv@chemcrys.cam.ac.uk**

– with the one-line message: **sendme depform**

or – on the World Wide Web, connect to the *CCDC* Home Page **hhtp://www.ccdc.cam.ac.uk/**

2) A table of final fractional atomic coordinates with standard uncertainties

3) Any calculated atomic coordinates (*e.g.* H-atoms)

4) A full list of bond lengths and angles with standard uncertainties

5) A full list of displacement parameters in the form of B_{ij} *or* U_{ij} (in Å^2 or pm^2)

Tables of structure factors (F_o, F_c) should not be submitted, but copies should be retained by the authors so that they may be made available to the referees *via* the Editorial Office if requested.

Authors are encouraged to submit all supplementary crystallographic data as an ascii (plain text) file on diskette, but hard copy will also be accepted. Multiple data sets for a given manuscript should be in a single file. This will minimize the chance that files will be misplaced or associated with the wrong manuscript. The individual structures in the combined file must be separated from each other by the sequence '#===END' at the beginning of a line. Authors must identify which manuscript the electronic file is associated with by entering the name of the manuscript at the top of the electronic file.

When the *CCDC* Deposition Form is used, the following footnote should be added to the manuscript:

'Crystallographic data (excluding structure factors) for the structure(s) reported in this paper have been deposited with the *Cambridge Crystallographic Data Centre* as supplementary publication No. CCDC-10/m. Copies of the data can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK. (fax: +44-(0)1223-336033 or e-mail: teched@chemcrys.cam.ac. uk).'

8. Proofs and Corrections

Authors will be provided with two sets of proofs, one of which should be returned to the editor within the indicated deadline.

Corrections of errors other than those due to the printers or editors will be charged. Standard correction marks should be used.

Together with the proofs the authors will receive a form for key words. The completed form must be returned with the proofs.

> Key words are entries in the annual subject index. Well-chosen key words will help a reader to find articles of potential interest. Key words should consist of not more than three words. Very general words or phrases (*e.g.* organic compounds, synthesis, instability, color, *etc.*) are clearly unsuitable as key words.

Appendix I. *Abbreviated Journal Titles*

A
Acc. Chem. Res.
Acta Chem. Scand., Ser. A/B
Acta Crystallogr., Sect. A/B
Adv. Mass Spectrom.
Adv. X-Ray Anal.
Agric. Biol. Chem.
Anal. Biochem.
Anal. Chem.
Anal. Chim. Acta
Angew. Chem.
Angew. Chem. Int. Ed.
Angew. Makromol. Chem.
Ann. Chim. (Fr.)
Ann. Chim. (Roma)
Arzneim.-Forsch.
Aust. J. Chem.

B
Ber. Bunsenges. Phys. Chem.
Ber. Dtsch. Chem. Ges.
Biochemistry
Biochem. Biophys. Res. Commun.
Biochem. J.
Biochem. Pharmacol.
Bull. Chem. Soc. Jpn.
Bull. Soc. Chim. Belg.
Bull. Soc. Chim. Fr.

C
Can. J. Biochem.
Can. J. Chem.
Carbohydr. Res.
Chem. Abstr.
Chem. Ber.
Chem. Eng. News
Chem. Eng. Sci.
Chem. Eng. (N.Y.)
Chem. Ind. (London)
Chem. Lett.
Chem. Pharm. Bull.
Chem. Phys. Lett.
Chem. Phys.
Chem. Rev.
Chem. Soc. Rev.
Chimia
Collect. Czech. Chem. Commun.
C.R. Acad. Sci., Ser. II/III

D
Dokl. Akad. Nauk SSSR

E
Electrochim. Acta
Eur. J. Biochem.
Eur. J. Pharmacol.
Experientia

F
Fresenius' J. Anal. Chem.

G
Gazz. Chim. Ital.

H
Helv. Chim. Acta
Heterocycles

I
Indian J. Chem., Sect. A/B
Inorg. Chem.
Inorg. Chim. Acta
Inorg. Nucl. Chem. Lett.
Int. J. Biochem.
Int. J. Chem. Kinet.
Int. J. Mass Spectrom. Ion Phys.

Int. J. Pept. Protein Res.
Int. J. Quantum Chem.
Izv. Akad. Nauk SSSR, Ser. Khim.

J
Jpn. J. Antibiot.
Jpn. J. Pharmacol.
J. Am. Chem. Soc.
J. Antibiot.
J. Appl. Chem. Biotechnol.
J. Appl. Crystallogr.
J. Appl. Electrochem.
J. Biochem.
J. Biol. Chem.
J. Chem. Educ.
J. Chem. Phys.
J. Chem. Soc., Chem. Commun.
J. Chem. Soc., Dalton Trans.
J. Chem. Soc., Faraday Trans. 1/2
J. Chem. Soc., Perkin Trans. 1/2
J. Chem. Thermodyn.
J. Chromatogr.
J. Chromatogr. Sci.
J. Electrochem. Soc.
J. Electron Spectrosc. Relat. Phenom.
J. Fluorine Chem.
J. Heterocycl. Chem.
J. Lipid Res.
J. Liq. Chromatogr.
J. Magn. Reson.
J. Med. Chem.
J. Mol. Spectrosc.
J. Organomet. Chem.
J. Org. Chem.
J. Pharm. Pharmacol.
J. Pharm. Sci.
J. Photochem.
J. Phys. Chem.
J. Prakt. Chem.
J. Radioanal. Chem.
J. Solid State Chem.
J. Solution Chem.
J. Steroid Biochem.

K
Khim. Prir. Soedin.

L
Liebigs Ann. Chem.
Lipids

M
Microchem. J.
Mikrochim. Acta
Mol. Pharmacol.
Mol. Phys.
Monatsh. Chem.

N
Nature (London)
Naturwissenschaften
Nouv. J. Chim.
Nucleic Acids Res.

O
Org. Magn. Reson.
Org. Mass Spectrom.

P
Pharmacology
Pharmacol. Res. Commun.
Photochem. Photobiol.
Phytochemistry
Planta Med.
Polym. J.
Pol. J. Chem.
Proc. Anal. Div. Chem. Soc.
Proc. Natl. Acad. Sci. U.S.A.
Pure Appl. Chem.

R
Radiat. Phys. Chem.
Recl. Trav. Chim. Pays-Bas

S
Science
Spectrochim. Acta, Part A/B
Synthesis
Synth. Commun.
Synth. Lett.

T
Talanta
Tetrahedron
Tetrahedron Lett.
Theor. Chim. Acta
Topics Curr. Chem.

V
Vitamins

Y
Yakugaku Zasshi

Z
Z. Anorg. Allg. Chem.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.
Z. Naturforsch., A/B/C
Z. Phys. Chem. (Leipzig)
Z. Phys. Chem. (Wiesbaden)
Zh. Neorg. Khim.
Zh. Obshch. Khim.
Zh. Org. Khim.

Appendix II. *Line Thickness and Size of Lettering for Original Drawings*

The thinnest lines in a printed figure or formula should not be narrower than 0.15 mm. The following table will serve as a guide in preparing original drawings.

Line thickness required [mm]

Format of original drawing [cm × cm]	Main part of drawing	Emphasized lines	Secondary lines
7.5 × 10.5	0.3–0.5	0.5–0.9	0.25–0.3
10.5 × 14.8	0.4–0.6	0.6–1.2	0.3 –0.4
14.8 × 21	0.6–0.9	0.9–1.8	0.5 –0.6
21 × 30.5	0.8–1.2	1.2–2.4	0.6 –0.8
30.5 × 42	1.0–1.5	1.5–3.0	0.8 –1.0

Distances between parallel lines or between letters should not be smaller than the line thickness.

The minimum height of lettering depends on the required linear reduction, as indicated in the following table.

Format of original drawing [cm × cm]	Height of capitals	
	Main lettering [mm]	Secondary lettering [mm]
7.5 × 10.5	3	2
10.5 × 14.8	4	2.5
14.8 × 21	6	4
21 × 30.5	8	5
30.5 × 42	10	6

Appendix III. *IUPAC Recommendations on Nomenclature, Symbols, and Terminology*

I. Nomenclature of Organic Chemistry

1. 'Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H; 1979 Edition' (The 'Blue Book'), IUPAC, Pergamon Press, Oxford, 1979.
2. 'A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993', Blackwell Scientific Publications, Oxford–London–Edinburgh–Boston–Melbourne–Paris–Berlin–Vienna.
3. 'Extension of Rules A-1.1 and A-2.5 Concerning Numerical Terms Used in Organic Chemical Nomenclature (Provisional)', *Pure Appl. Chem.* **1983,** *55,* 1463.
4. 'Revision of the Extended *Hantzsch-Widman* System of Nomenclature for Heteromonocycles', *Pure Appl. Chem.* **1983,** *55,* 409.
5. 'Treatment of Variable Valence in Organic Nomenclature (Lambda Convention) (Recommendations 1983)', *Pure Appl. Chem.* **1984,** *56,* 769.
6. 'Glossary of Terms Used in Physical Organic Chemistry', *Pure Appl. Chem.* **1983,** *55,* 1281.
7. 'Nomenclature for Straightforward Transformations (Provisional)', *Pure Appl. Chem.* **1981,** *53,* 305.
8. 'Extension of Rules A-1.1 and A-2.5 Concerning Numerical Terms Used in Organic Chemical Nomenclature', *Pure Appl. Chem.* **1986,** *58,* 1693.
9. 'Glossary of Terms Used in Photochemistry (Recommendations 1988)', *Pure Appl. Chem.* **1988,** *60,* 1055.
10. 'Names for Hydrogen Atoms, Ions, and Groups, and Reactions Involving Them (Recommendations 1988)', *Pure Appl. Chem.* **1988,** *60,* 1115.
11. 'Nomenclature for Cyclic Organic Compounds with Contiguous Formal Double Bonds (the δ-Convention) (Recommendations 1988)', *Pure Appl. Chem.* **1988,** *60,* 1395.
12. 'System for Symbolic Representation of Reaction Mechanisms (Recommendations 1988)', *Pure Appl. Chem.* **1989,** *61,* 23.
13. 'Nomenclature for Organic Chemical Transformations (Recommendations 1988)', *Pure Appl. Chem.* **1989,** *61,* 725.
14. 'Biotransformation – a Useful Tool in Organic Chemistry', *Pure Appl. Chem.* **1990,** *62,* 753.
15. 'Revised Nomenclature for Radicals, Ions, Radical Ions, and Related Species (Recommendations 1993)', *Pure Appl. Chem.* **1993,** *65,* 1357.
16. 'Glossary of Terms Used in Physical Organic Chemistry (Recommendations 1994)', *Pure Appl. Chem.* **1994,** *66,* 1077.
17. 'Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure (Recommendations 1995)', *Pure Appl. Chem.* **1995,** *67,* 1307.

II. Biochemical Nomenclature

1. 'Biochemical Nomenclature and Related Documents', IUB, 3rd Edition, The Biochemical Society, London, 1978.
2. 'Nomenclature and Symbolism for Amino Acids and Peptides (Recommendations 1983)', *Pure Appl. Chem.* **1984,** *56,* 595.
3. 'Abbreviated Nomenclature of Synthetic Polypeptides (Polymerized Amino Acids)', *Pure Appl. Chem.* **1973,** *33,* 437.
4. 'Abbreviations and Symbols for Description of Conformation of Polypeptide Chains (Rules Approved 1974)', *Pure Appl. Chem.* **1974,** *40,* 291.
5. 'Tentative Rules for Carbohydrate Nomenclature, Part. I, 1969', *Biochemistry* **1971,** *10,* 3983, 4995; *Biochim. Biophys. Acta* **1971,** *244,* 223; *Eur. J. Biochem.* **1971,** *21,* 455, and **1972,** *25,* 4; *Biochem. J.* **1971,** *125,* 673.
6. 'Nomenclature of Unsaturated Monosaccharides (Provisional)', *Pure Appl. Chem.* **1982,** *54,* 207.
7. 'Nomenclature of Branched-Chain Monosaccharides (Provisional)', *Pure Appl. Chem.* **1982,** *54,* 211.
8. 'Conformational Nomenclature for Five- and Six-Membered Ring Forms of Monosaccharides and their Derivatives (Provisional)', *Pure Appl. Chem.* **1981,** *53,* 1901.
9. 'Polysaccharide Nomenclature (Provisional)', *Pure Appl. Chem.* **1982,** *54,* 1523.
10. 'Abbreviated Terminology of Oligosaccharide Chains (Provisional)', *Pure Appl. Chem.* **1982,** *54,* 1517.

11. 'Symbols for Specifying the Conformation of Polysaccharide Chains (Provisional)', *Pure Appl. Chem.* **1983,** *55,* 1269.
12. 'Nomenclature of Cyclitols', *Pure Appl. Chem.* **1974,** *37,* 283.
13. 'Abbreviations and Symbols for Nucleic Acids, Polynucleotides, and their Constituents (Rules Approved 1974)', *Pure Appl. Chem.* **1974,** *40,* 277.
14. 'Abbreviations and Symbols for the Description of Conformations of Polynucleotide Chains (Provisional)', *Pure Appl. Chem.* **1983,** *55,* 1273.
15. 'Nomenclature of Tetrapyrroles (Recommendations 1986)', *Pure Appl. Chem.* **1987,** *59,* 779.
16. 'Nomenclature of Corrinoids', *Pure Appl. Chem.* **1976,** *48,* 495.
17. 'Nomenclature of Steroids (Recommendations 1989)', *Pure Appl. Chem.* **1989,** *61,* 1783.
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Appendix IV. *Some Symbols and Abbreviations Used by HCA*

Designation	Symbol	Remarks
Amount-of-substance concentration or 'molarity'[a])	M	in mol/dm^3; ex.: 1M NaOH
Molality[a])	*m*	in mol/kg; ex.: 1*m* HCl
Normality[a])	N	in equiv./dm^3; ex.: 1N H_2S
Percentage by mass	%	*e.g.* 15%
Percentage by volume	% (*v*/*v*)	*e.g.* 20% (*v*/*v*)
Melting point	m.p.	*e.g.* m.p. 157–158°
Boiling point	b.p.	*e.g.* b.p. 111–112°
Boiling point under a certain pressure	b.p./Torr	*e.g.* b.p. 65°/4 Torr
Freezing point	f.p.	*e.g.* f.p. 3°
Refractive index	*n*	*e.g.* $n_d^{20} = 1.643$
Relative density	*d*	*e.g.* $d_4^{20} = 1.1811$
Optical rotation[b])	α	*e.g.* $\alpha_D^{25} = 0.73$ ($l = 0.1$, neat)
Specific optical rotation[b])	$[\alpha]$	*e.g.* $[\alpha]_D^{25} = 108$ ($c = 3.42$, $CHCl_3$)
Molecular optical rotation[b])	$[M]$	*e.g.* $[M]_{598}^{23} = 380$ ($c = 1.52$, H_2O)
Thin-layer chromatography	TLC	
Gas-liquid chromatography	GLC	
Liquid chromatography	LC	
Column chromatography	CC	
High-pressure (performance) liquid chromatography	HPLC	
Paper chromatography	PC	
Ultraviolet	UV	
Visible	VIS	
Circular dichroism	CD	
Optical rotatory dispersion	ORD	
Infrared (absorption)	IR	
Nuclear magnetic resonance of ^1H	^1H-NMR	
Nuclear magnetic resonance of ^{13}C	^{13}C-NMR	
Electron paramagnetic resonance	EPR	
Electron spin resonance	ESR	
Mass spectrum	MS	
Photoelectron spectroscopy	PES	
X-Ray photoelectron spectroscopy	XPES, ESCA	
Shoulder	sh	
Broad	br.	
Strong IR absorption	*s*	
Medium IR absorption	*m*	
Weak IR absorption	*w*	
Singlet	*s*	
Doublet	*d*	
Triplet	*t*	
Quadruplet	*q*	
Quintuplet	*quint.*	
Sextuplet	*sext.*	
Septuplet	*sept.*	
Multiplet	*m*	

[a]) For a comprehensive discussion on the usage of the terms 'equivalent' and 'normal', see IUPAC, *Pure Appl. Chem.* **1978,** *50*, 325.

[b]) The symbol *c* is used in connection with the specific optical rotation $[\alpha]$; it is defined as mass of substance (in g) in 100 ml of solution. The quantities *l* and *d* in $[\alpha] = 100 \cdot \alpha / l \cdot c$ or $[\alpha] = \alpha / l \cdot d$ are given in dm and g/ml (kg/m^3), respectively.

Appendix V. *Some Acceptable Non-SI Units*

Physical quantity	Name of unit	Symbol of unit
Length	Ångström	Å
	Bohr radius	a_o
Volume	Liter	l
	Milliliter	ml
	Microliter	µl
Time	Minute	min
	Hour	h
	Day	d
Frequency	Hertz	Hz
	Megahertz	MHz
Mass	Gram	g
	Milligram	mg
	Microgram	µg
Pressure	Bar	bar
	Millibar	mbar
	Torr	Torr
Energy	Electronvolt	eV
	Hartree	H_a or E_a
Temperature	Degree Celsius	°C
Dipole moment	Debye	D