HELVETICA CHIMICA ACTA

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The journal *Helvetica Chimica Acta* (*HCA*) invites selected original and significant contributions of fundamental research in all branches of the theory and practice of chemistry. The critical selection criteria are originality and quality of the work, as well as the breadth of interest to readers and subscribers.

Contributions are considered from non-members as well as members of the *Swiss Chemical Society*. Manuscripts may be submitted for publication as *Articles*, *Notes*, and *Preliminary Communications*; *Review Articles* are also considered for publication in *HCA*.

Contents of manuscripts submitted to *HCA* must not have been published previously, except in the form of a brief preliminary communication, nor have been submitted to another journal.

Manuscripts should be submitted **either** in *triplicate*, together with the *electronic version* and a transmittal letter signed by the author to whom correspondence should be addressed, **or** *only electronically* (vhca@vhca.ch) as attachment (text and graphic files) to:

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2. Preparation of Manuscripts

2.1. ***General Considerations.*** Careful preparation of the manuscript and adherence to the format and conventions of *HCA* as laid down in these *Instructions for Authors* will facilitate rapid publication. Authors should consult recent issues of *HCA* for examples.

Manuscripts may be submitted in English, German, French, or Italian. Manuscripts must be prepared with a word processor and be printed *double-spaced* to allow for editorial markings. 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.

Pages should be numbered consecutively beginning with the title page. References, tables, scheme and/or 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.

A representative structural formula or scheme should be provided for the Table of Contents. The *maximum* available place for this graphical abstract is 5×11 cm.

Authors who are not fully fluent in English are strongly advised to seek assistance from a fluent colleague when preparing a manuscript. In all cases, it is wise to consult a standard manual of style (*e.g.*, 'The ACS Style Guide: A Manual for Authors and Editors', 3rd edn., Eds. A. M. Coghill, L. R. Garson, American Chemical Society, Oxford University Press, Oxford, New York, 2006, or W. Strunk Jr., E. B. White, 'The Elements of Style', 4th edn., Prentice Hall, New York, 1999 (also found at *http://www.bartleby.com/141/index.html*)). Manuscripts containing grammatical and/or stylistic deficiencies are handicapped during the review and editorial processes, leading to *rejection* or *significantly longer publication times.*

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- Boldface: headings, designated numbers of chemical compounds.
- Italic: subheadings, configurational prefixes ((*R*)-, (*S*)-, *cis*-, *trans*-, *etc.*), Latin words or abbreviations, trade names of chemical compounds (first letter should be capitalized), names of authors if mentioned in the text.
- Small capital: symbols of molar and normal concentrations (M and N), D and L, the names of the discoverer in the nomenclature of genera, species, or varieties.
- Boldface italic: the italicized terms and prefixes in headings.

Special characters not available in the word-processing program should be clearly drawn in ink and explained unambiguously in the margin on first appearance.

2.2. *Title Page.* For the layout of the title page, a current issue of *HCA* should be consulted.

Attention is drawn to the following points:

a) The title of a manuscript, being of greatest importance for attracting readers' interest and for information retrieval, should clearly and accurately provide information on the content and emphasis of the work. The use of abbreviations, symbols, chemical formulae, and references in a title is strongly discouraged. 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(es) of the contributing laboratory or laboratories. The author to whom correspondence and/or inquiries should be directed should be indicated with an asterisk (*). Footnotes may be added to indicate the present mailing address(es) of the author(s). The corresponding author's mailing address, phone number, fax number, and e-mail address should also be included.

2.3. *Abstract.* The second page of the manuscript should be reserved for an abstract in English, independent of the language of the main text. If this is German, French, or Italian, the abstract should be preceded by an English translation of the title. ***The abstract, stating briefly the purpose of the research (if not clear from the title), the principal results, and major conclusions, should be self-explanatory and intelligible without reference to the text.*** References to structural formulae, *Tables*, *Schemes*, and *Figures*, by number, may be made in the abstract. For a typical contribution, an 80- to 200-word abstract is usually adequate.

2.4. *Keywords.* Keywords are used as entries in the annual subject index and will be published together with the Abstract on *http://wileyonlinelibrary.com/journal/hca*. Well-chosen keywords will help a reader to find articles of potential interest. Individual keywords should not consist of more than three words. Very general words or phrases (*e.g.*, organic compounds, synthesis, instability, color, *etc.*) are unsuitable as keywords. Preferably not more than five keywords should be provided for a contribution.

2.5. *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*).

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 accepted. *b*) Only the initials of first and middle names should be given. *c*) The name of the journal and volume number cited should be given in italics [1]. *d*) Composite references may be used, instead of a series of individual ones [2]. The use of the Latin terms *ibid.* and *idem* is no longer allowed, since these are not compatible with electronic information-retrieval systems [3]. When a part of a composite reference is cited individually in the text, the parts of the composite reference may be specified by a), b), *etc.* [4a][4b]. *e*) In references described as 'personal communications', an affiliation

should follow the name(s) of the person(s) cited [5]. *f*) Descriptions such as 'for a review, see . . .' should be included in the body of the text and not as part of the reference.

Examples of references to book chapters [6], books [7], patents [8], computer programs [9], and Ph.D. theses [10] are also given.

REFERENCES

[1] M. Barbero, I. Degani, S. Dughera, R. Fochi, L. Piscopo, *J. Chem. Soc., Perkins Trans. 1* **1996**, 289.
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[8] T. Kamata, N. Wasada, Jap. Pat. 2-204469, 1990, p. 381–384.
[9] G. M. Sheldrick, SHELXL97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.
[10] B. R. Peterson, Ph.D. Thesis, University of California at Los Angeles, 1994.

In the text, reference to author(s) of cited works should be made without giving initials, *e.g.*, '. . . as shown by *Kamata* and *Wasada* [8]'. If the reference carries the names of three or more authors it should be quoted as '*Barbero et al.* [1]', if *Barbero* is the first author, or as '*Piscopo* and co-workers [1]', if *Piscopo* is the senior author.

2.6. *Footnotes.* Footnotes, *i.e.*, explanations or comments on the text, should be kept to a minimum. Each one should be indicated in the manuscript by a superscripted number followed by a closing parenthesis, *e.g.*, '. . . is implied[1]), otherwise . . .', and numbered sequentially throughout the manuscript. Each footnote should be typed ***double-spaced*** at the bottom of the page of the manuscript in which it is first mentioned. Footnotes must not be included with the references.

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2.8. *Structural Formulae, Schemes, and Figures.* Laser printouts, 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 on A4 paper are preferred, and they must contain all

necessary symbols and lettering, *i.e.*, they must be usable without additional artwork by the *HCA* printers.

Line thickness, line spacing, and, especially, the size of all the necessary symbols and lettering should be planned for optimal legibility after photoreduction to 12.5-cm width. All atom labels and text should be in 'plain' style (lightface), and compound numbers should be in boldface type. 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 boldface key numbers; compounds mentioned only in the text should be referred to by name.

Good-quality representations of graphical material are a prerequisite for publication in *Helvetica Chimica Acta*. Please consult the *IUPAC Recommendations on Graphical Representation of Stereochemical Configuration and Standards for Chemical Structure Diagrams* (see *Appendix II*, *VII Miscellaneous*, *6* and *7*). If, after acceptance of a manuscript for publication, further changes in the graphical representations need to be executed by the Editorial staff, the corresponding expenses will be charged to the author(s).

Currently, the following chemical drawing packages are acceptable: *ChemDraw* up to version 12.0, *Isis/Draw* up to version 2.5, or *ACD/ChemSketch* up to version 12.5. For style files and drawing settings, please visit the following internet page: *http//www.helvchimacta.ch/chemicaldrawing.htm*.

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proposed by *IUPAC* (*cf. Pure Appl. Chem.* **1979**, *51*, 1) are recommended. Fractional expressions should be written with a slash, *e.g.*, *hν*/*kT*.

3. Electronic Submission of Manuscripts

An electronic version of the manuscript should also be submitted. Submissions not provided in electronic form may face significant delays in publication. *The following word-processing packages are currently accepted*: PC: *MS Word* (up to version 2010); *Macintosh*: *MS Word* (up to version 2011). Publication of manuscripts prepared with these software packages may be facilitated, if the following guidelines are adhered to. Failure to adhere to these instructions may prevent all or part of the material supplied on disk from being used in production.

A hardcopy (in *triplicate*) of the manuscript is required for review. Electronically saved material should accompany the manuscript. The electronic version ***must*** exactly match the version of the hardcopy.

When preparing a manuscript, use the document mode or its equivalent in the word-processing program; *i.e.*, do not save files in 'Text Only' (ASCII) mode. If a non-Western version of the word-processing software was used to prepare the manuscript, save the file in Rich-Text Format (RTF). Do not include any page-layout instructions such as placement information for graphics in the file. The text should be left-justified, and automatic end-of-line hyphenation should be turned off. Use carriage returns only to end headings and paragraphs, not to break lines of text. Do not insert spaces before punctuation. References must conform to the format described above and printed in the journal. Ensure that all characters are correctly represented throughout the manuscript: for example, 1 (one) and l (ell), 0 (zero) and O (Oh), X (ex) and × (times sign). Check the final copy carefully for consistent notation and correct spelling. Check the disk with a virus-detection program. Disks containing viruses will not be processed. Label the disk with the manuscript name and the name of corresponding author. Additionally, platform, version of software used, and file names should be provided.

All text (including the title page, abstract, all sections of the manuscript, figure captions, scheme or chart titles and footnotes, and references) and tabular material should be in one file, with the complete text first, followed by the tabular material. It is best to use the fonts '*Times New Roman*' or '*Times*', '*Symbol*', and '*Arial*' or '*Helvetica*'. Some other fonts, particularly those that do not come bundled with the system software, may not translate properly. Ensure that all special characters (*e.g.*, Greek characters, math symbols, *etc.*) are present in the body of the text as characters and not as graphical representations. Tables created with a word processor's table format feature are preferred over those prepared in text mode. Ensure that each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row.

Graphics, *e.g.*, figures, schemes, *etc.* should be provided on a separate diskette or CD in the original file format and as TIFF files at a resolution of at least 300 dpi. The file name for each image should be descriptive for the graphic. Since TIFF files are rather large, they may also be compressed (as zip files).

4. Nomenclature

All new compounds should be named in accordance with *IUPAC* rules (*cf. Appendix II*). As an additional guideline, the *Index Guide of Chemical Abstracts* should be consulted. The use of *ACD/Name* (version 12.5) is recommended. 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. An *ad hoc* abbreviation may be used for a name or formula that occurs repeatedly. This has to be clearly defined, *e.g.*, tetrahydrocannabinol (THC).

Different alkyl or arylalkyl radicals should be designated with superscripted numbers: R^1, R^2, R^3, *etc.* (Subscripts are used only to denote stoichiometry.) 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).

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

5. 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 IV* are acceptable.

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

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

It is the results of crystal-structure determinations that are of prime interest to readers of *HCA*. A detailed description of the experiment is not usually necessary, and only the pertinent crystallographic data need to be summarized in the experimental section. However, the full crystallographic data must be deposited in one of the crystallographic databases (see *d* below) ***before*** the manuscript is submitted. In addition, authors must validate their crystallographic data (see *c* below) and include the Validation Report with their manuscript. The manuscript will not be distributed to the referees until the database deposition numbers and Validation Reports for the reported crystal structures have been provided.

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

A labeled view of the molecule with ***displacement ellipsoids, not arbitrary spheres***, will usually suffice, unless the authors specifically wish to discuss particular aspects of the structure or the experiment.

A brief description of the structure or any unusual features therein and a table of significant bond lengths, angles, or torsion angles may be given where appropriate to the discussion.

Full tables of refined atomic coordinates, bond lengths and angles, and related information will only be printed when *specifically* requested by the authors, and when 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
– Crystal size
– 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 $R(F)$ for the $I > n\sigma(I)$ reflections, wR (on F or F^2) for all reflections used in the refinement, and S (goodness-of-fit)
– 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

c) Validation of Crystallographic Data (to be done before submission of the manuscript)

In order to reduce the likelihood of incorrect or substandard crystal structures being reported, authors must test the validity of their crystal-structure determinations prior to submission of their manuscript. The CIF [3]) for each structure in the paper can be uploaded to the IUCr's CHECKCIF facility at *http://journals.iucr.org/services/cif/checking/checkform.html* or validated locally with the program PLATON (down-

[3]) Details concerning the Crystallographic Information File (CIF) format are available from *Acta Crystallogr., Sect. A* **1991**, *47*, 655 or *http://www.iucr.org/iucr-top/cif/index.html.*

loadable from *http://www.cryst.chem.uu.nl/platon/*). Both of these validation methods generate a Validation Report. Authors should examine the Validation Reports to ensure that no serious oversight has occurred with their crystal structure determinations (*e.g.*, incorrect space group, seriously deficient data quality or structural model) and take appropriate corrective action when required. A copy of the final Validation Report for each structure in the paper must be submitted with the manuscript, and any unresolved serious validation issues should be commented upon.

d) Deposition of Crystallographic Data (to be completed before submission of the manuscript)

Prior to submission of a manuscript, all crystallographic data must be deposited electronically in CIF format with the appropriate crystallographic database so that the referees can access the data.

The crystallographic data for ***organic and organometallic*** compounds should be deposited with the *Cambridge Crystallographic Data Centre* (*CCDC*) (see: *http://www.ccdc.cam.ac.uk*). Send your data in CIF format (excluding structure factors) by e-mail to *deposit@ccdc.cam.ac.uk*. The *CCDC* will provide the authors with one deposition number for each structure by return e-mail. These deposition numbers should be included as a footnote in the manuscript by using the following standard text:

> 'CCDC-…… contains the supplementary crystallographic data for this paper. These data can be obtained free of charge *via* http://www.ccdc.cam.ac.uk/data_request/cif.'

The data for ***inorganic*** compounds should be deposited with the Fachinformationszentrum Karlsruhe (see: *http://www.fiz-informationsdienste.de/en/DB/icsd/depot.html*). Send your CIF by e-mail to *crysdata@fiz-karlsruhe.de*. A CSD number will be notified by return e-mail. The CSD number should be included as a footnote in the manuscript by using the following standard text:

> 'Further details of the crystal structure investigation(s) may be obtained from the Fachinformationszentrum Karlsruhe, Informationsdienste, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany, on quoting the depository number(s) CSD.…'

7. Proofs and Corrections

The corresponding authors will be provided with PDFs of the galley proof and of the edited manuscript *via* e-mail. Amendments and/or additions must be returned to the editor within 7 days upon receipt of the e-mail. The author is solely responsible for checking the proofs.

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

A total of 30 reprints will be provided free of charge to the corresponding author. Additional reprints and/or a high-resolution PDF may be requested as indicated on the title page of the galley proof.

Appendix I. *Selected Journal Abbreviations*

A

Acc. Chem. Res.
Acta Chem. Scand., Ser. A/B
Acta Crystallogr., Sect. A/B/C/D/E/F
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. (Cachan, Fr.)
Ann. Chim. (Rome)
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. Biodiversity
Chem. Commun. (Cambridge, U.K.)
Chem. Eng. News
Chem. Eng. Sci.
Chem. Eng. (N. Y.)
Chem. – Eur. J.
Chem. Ind. (London)
Chem. Lett.
Chem. Pharm. Bull.
Chem. Phys.
Chem. Phys. Lett.
Chem. Rev. (Washington, DC, U.S.)
Chem. Soc. Rev.
Chimia
Collect. Czech. Chem. Commun.
C. R. Acad. Sci., Ser. II/III

D

Dalton Trans.
Dokl. Akad. Nauk SSSR

E

Electrochim. Acta
Eur. J. Biochem.
Eur. J. Inorg. Chem.
Eur. J. Org. Chem.
Eur. J. Pharmacol.
Experientia

F

Faraday Trans.
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

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. 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. Nat. Prod.
J. Organomet. Chem.
J. Org. Chem.
J. Pharm. Pharmacol.
J. Pharm. Sci.
J. Photochem.
J. Phys. Chem. A/B/C
J. Prakt. Chem.
J. Radioanal. Chem.
J. Solid State Chem.
J. Solution Chem.
J. Steroid Biochem.
Jpn. J. Antibiot.
Jpn. J. Pharmacol.

K

Khim. Prir. Soedin.

L

Liebigs Ann. Chem.
Lipids

M

Microchem. J.
Microchim. 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

Perkin Trans. 1/2
Pharmacology
Pharmacol. Res. Commun.
Photochem. Photobiol.
Phytochemistry
Planta Med.
Polym. J. (Tokyo, Jpn.)
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 (Washington, DC, U.S.)
Spectrochim. Acta, Part A/B
Synthesis
Synth. Commun.
Synlett

T

Talanta
Tetrahedron
Tetrahedron Lett.
Theor. Chim. Acta
Top. Curr. Chem.

V

Vitamins

Y

Yakugaku Zasshi

Z

Z. Anorg. Allg. Chem.
Z. Kristallogr., Kristallogeom., 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. *IUPAC Recommendations on Nomenclature, Symbols, and Terminology*

Visit also the following internet page: *http://www.chem.qmul.ac.uk/iupac/.*

I. Nomenclature of Organic Chemistry

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Appendix III. *Some Symbols and Abbreviations Used by HCA*

Designation	Symbol	Remarks
Amount-of-substance concentration or 'molarity' [a])	M	in mol/dm^3, *e.g.*, 1M NaOH
Molality [a])	*m*	in mol/kg; *e.g.*, 1 *m* HCl
Normality [a])	N	in equiv./dm^3; *e.g.*, 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.*, $\alpha = 0.73$ ($l = 0.1$, 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 ^{1}H	^{1}H-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 *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 IV. *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	° or °C
Dipole moment	Debye	D