The Organic Chemist's Desk Reference

A COMPANION VOLUME TO THE DICTIONARY OF ORGANIC COMPOUNDS, SIXTH EDITION

P.H. Rhodes

CHAPMAN & HALL
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DICTIONARY OF ORGANIC COMPOUNDS, Sixth Edition

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With contributions from other DOC editors and contributors
Hazard and toxicity information by R. Purchase

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Preface

Organic chemistry is literally a vital science, in two respects. First, it controls the functioning of living organisms through the operation of the complex series of reactions that power them. The details of these reactions are studied in tandem with the sister discipline, biochemistry. Secondly, an enormous range of organic reactions are carried out daily throughout the world, some on a very large scale, producing the fuels, materials, medicines, insecticides and other essential organic compounds in daily use.

Organic chemists are sometimes accused of being insular, but success in organic chemistry needs a lively appreciation of the other sciences – and not just other branches of chemistry. An assertion perhaps closer to the truth is that in order to make a success of organic chemistry, the practitioner needs to know so many specialist facts and methods that the subject can be daunting to a non-specialist.

Anything that helps the organic chemist, or any other scientist using organic chemical information, to access rapidly as much of this knowledge as possible is to be welcomed. There are many review series and reference works in daily use throughout the world, and one of these is the *Dictionary of Organic Compounds* (DOC), with which some of us have been associated for many years. As part of the major revision of this work that has taken place for the preparation of the new Sixth Edition, the idea arose of a slender companion volume that would include a wide variety of the miscellaneous facts that organic chemists constantly need but which would be out of place in DOC 6 itself.

We make no apology for the fact that one of the functions of this volume is to publicise the new DOC 6 and to help users to get the most out of it. But in addition they will find collected here a mass of useful up-to-date information, which is often irritatingly scattered and difficult to locate, including details of the content of most of the other major reference sources.

This companion volume is published both in hard covers as part of the DOC 6 set, and separately as a modestly priced paperback, which is available in bulk to teachers and research directors. We are confident that it will be widely used, and expect that further editions will be called for: any suggestions concerning data for future inclusions will be welcomed and should be addressed to the DOC editors at Chapman & Hall.

The Editorial Board
J.I.G. Cadogan, S.V. Ley
G. Pattenden, R.A. Raphael
C.W. Rees

1 History of the *Dictionary of Organic Compounds* (DOC)

The First Edition of DOC, edited by Sir Ian Heilbron and H.M. Bunbury, was published in 1934 in three volumes. DOC was periodically updated, leading to the Fourth Edition (1964), which was updated by annual supplements in the years 1965–79. For the Fifth Edition (1982), DOC was completely revised and transferred onto a fielded database. This database became the Chapman & Hall Chemical Databank (CHCD), which is now the basis for the publication of not only DOC, but also other chemical dictionaries such as the *Dictionary of Natural Products* (DNP) and the *Dictionary of Organometallic Compounds*, which have resulted from the subsequent considerable enhancement of the database. A CD-ROM version of DNP was released in 1992 and of DOC in 1993.

Sir Ian Morris Heilbron (1886–1959) was an organic chemist distinguished for his work on natural products. Born in Glasgow, he studied chemistry there at the Royal Technical College (now the University of Strathclyde) before taking his Ph.D. degree at Leipzig, where he studied under Hantzsch. In 1909 he returned to the Royal Technical College, where he was a lecturer until the outbreak of World War I. He served with distinction as an officer during the war, being awarded the DSO and promoted to Lieutenant-Colonel, finishing as Assistant Director of Supplies at GHQ, Salonika. After the war he worked for a short time at the British Dyestuffs Corporation in Manchester, which became part of ICI, before returning to the Royal Technical College as Professor of Chemistry. He later held Chairs at Liverpool (1920–33), Manchester (1933–38) and Imperial College (1938–49). During World War II he acted as a scientific adviser to the Ministry of Production, and he played a leading part in the introduction of DDT. He retired from academic life in 1949 and was appointed the first Director of the Brewing Industry Research Foundation, where he remained until his death in 1959.

Hugh Mills Bunbury was born on 21 September 1889. During World War I he served in the City of London Regiment (Royal Fusiliers) and was attached to the Ministry of Munitions. In 1919 he joined the British Dyestuffs Corporation in Manchester, which became part of ICI, where he became a colleague of Heilbron's. He later trained as a barrister, retiring from ICI in 1967. He wrote *The Industrial Applications of Coal Tar Products* with A. Davidson (1925), *The Destructive Distillation of Wood* (1923) and, much later, edited *Chemists and the Law*, published by E & FN Spon in 1967. He died on 17 May 1972.

The original proposal for a *Dictionary of Organic Compounds* was sent to the publishers by Bunbury in about 1931, and the First Edition was put together largely by Heilbron's research groups in Liverpool and Manchester.

1.1 The Chapman & Hall Chemical Databank and the Sixth Edition of DOC

The Chapman & Hall Chemical Databank, from which DOC is produced, is a selected and carefully edited resource containing chemical and physical data together with key literature references and structural information for approximately 300 000 chemical substances. The database was originally set up to produce the Fifth Edition of DOC, which was published in 1982. It has subsequently been considerably expanded to produce various further dictionaries, notably:

- *Dictionary of Organometallic Compounds* (First Edition 1984; Second Edition 1994)
- *Dictionary of Organophosphorus Compounds* (1988)
- *Dictionary of Drugs* (1990)
- *Dictionary of Inorganic Compounds* (1992)
- *Dictionary of Analytical Reagents* (1993)
- *Dictionary of Natural Products* (1994)

The new, Sixth Edition of DOC (1995) is the second to be produced from the database. Each of the main

dictionaries is continually updated. In print format, an annual Supplement is produced for each Dictionary.

Since 1993, these dictionaries have also been available in CD-ROM format, which features text searching and display by Headfast software provided by Head Software International, and substructure searching using PsiBase from Hampden Data Services. The two packages function on the same disk and are seamlessly linked to provide very flexible searching of the database by text, structure or a combination of both. The three main CD-ROM dictionaries are available on subscription, which provides a complete update every six months; the *Dictionary of Analytical Reagents* and the *Dictionary of Drugs* are available as one-off purchases.

1.2 The content of DOC 6

Considerable expansion of the databank that supports DOC has taken place since the Fifth Edition Main Work was published in 1982. Some reorganisation of the content of DOC has taken place in the new Sixth Edition, most notably concerning the coverage of natural products.

Natural products

In the late 1980s it was decided to publish a separate *Dictionary of Natural Products*, which would have the aim of being a comprehensive record of all known natural substances. DOC 6 therefore contains fewer natural product entries than DOC 5 but with a more rational focus, giving (sometimes abbreviated) entries only for the most widespread, practically important and structurally typical natural products. The *Dictionary of Natural Products* (published 1994) and its supplements (like DOC, available also in substructure-searchable CD-ROM format) gives a comprehensive coverage of the nearly 100 000 natural products now known.

Drugs

Similarly, DOC 6 focuses on a limited coverage of the most important drugs in common use: in 1996, DOC will be joined by a *Dictionary of Pharmacological Agents*, giving a much wider coverage, including substances of pharmaceutical interest that are not yet marketed.

Organometallics

DOC 5 contained a very limited number (about 500) of entries concerning the most fundamental organometallic structures, e.g. ferrocene. This coverage was discontinued with the compilation of the much more comprehensive *Dictionary of Organometallic Compounds* (First Edition 1984; Second Edition 1994). In this edition of DOC there are no entries for true organometallic compounds, but a good coverage of the organic compounds of boron and silicon, especially those with synthetic applications.

Increased coverage of core compounds

DOC 5 contained information on approximately 90 000 compounds, including numerous natural products, whereas DOC 6 documents 160 000 substances, with only restricted natural product coverage. Therefore, it will be clear to users that there has been a substantial increase, about 250%, in the fundamental starting materials, reagents and interesting target molecules that are the categories of compound of most interest to mainstream organic chemists, particularly those involved in synthesis. In order to ensure that this coverage corresponds as closely as possible to users' needs, the literature has been carefully reviewed to mid-1994.

2 User Guide to DOC

2.1 Using DOC 6

As with previous editions, the arrangement of entries is alphabetically by DOC Name. Thus, in cases where there is no possible ambiguity about the name, the compound can be located immediately without using the index. However, the majority of even quite simple organic compounds have at least two completely valid names (e.g. methylbenzene/toluene), and therefore, if a compound cannot be located immediately, the Name Index should be used. This includes all DOC Names and alternative names given throughout the DOC, including those applicable to derivatives. A Molecular Formula Index and CAS Registry Number Index are also provided.

Each entry is numbered to assist its ready location. The DOC Number consists of a letter of the alphabet, a supplement number, followed by a five-digit number. In the 'Main Work' volumes the first digit is invariably 0; entries in the First Supplement will carry a first digit 1; entries in the Second Supplement will carry the first digit 2; and so on. All index entries refer to the DOC Number. Each index is described in detail in the appropriate volume.

Many compounds appear as derivatives of parent compounds; compounds such as ethers, esters and *N*-methyl derivatives, if they cannot be located immediately, should be looked for (a) under the parent, (b) using the Name Index (in which all names of derivatives appear) or (c) using the Formula Index (which includes molecular formulae for all derivatives except those of a characterisation nature such as 2,4-dinitrophenylhydrazones).

2.2 Compound selection policy

2.2.1 General

Many thousands of new entries have been added to the new edition, and extensive reviews have been carried out of suitable sources to ensure that as far as possible the needs of all potential users of DOC have been taken into account. In general, DOC 6 covers the following classes of compounds:

- The basic fundamental organic compounds of simple structure that are frequently required as starting materials, and which have usually been the subject of extensive physicochemical study.
- The most important and widespread natural products. (The *Dictionary of Natural Products* provides comprehensive coverage of natural products, including more extensive entries for many of those which have DOC 6 entries.)
- Compounds with a well established use, e.g. pesticides and drugs in current use.
- Laboratory reagents and solvents.
- Other compounds with interesting chemical, structural or biological properties, including 'intriguing' molecules that have been specially synthesised in order to investigate their chemical and physical properties.

This coverage has been especially reviewed and enhanced for the new edition, and users should find that, for the majority of queries, it corresponds to their needs. The extensive inclusion of further orientating information about the compounds covered, such as CAS Names and CAS Registry Numbers, makes it easier to carry out a deeper search if more extensive information is needed about a particular compound.

The Editors are always pleased to receive comments on the selection policy, and in particular to receive specific suggestions for compounds or groups of compounds for inclusion.

2.2.2 Derivatives

Some types of compound are usually treated as derivatives of parent compounds, for example:

- Hydrates, complexes (e.g. picrates).
- Salts and quaternary salts, e.g. hydrochlorides and methobromides.
- Classical organic derivatives; for example, entries for esters, acid chlorides, amides and nitriles will be found under the parent acid unless they are

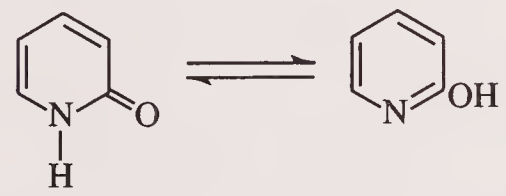
particularly important compounds in their own right, justifying their own entry.

All important derivatives occur in the Formula Index and can be traced in that manner.

2.2.3 Tautomerism in DOC 6

For the Sixth Edition of DOC the presentation of information on tautomeric compounds has been improved and standardised.

The commonest type of tautomerism encountered is the NH ⇌ OH equilibrium shown by many heterocyclic compounds, e.g. 2(1*H*)-pyridinone ⇌ 2-pyridinol (2-hydroxypyridine):



The position of equilibrium for a particular compound depends on various factors, but in general the NH form predominates for most heterocyclic compounds under most conditions. Simple derivatives may be either: (a) derivatives that are themselves capable of tautomerism, e.g. hydrochloride, *N*-oxide; (b) derivatives of the NH form, e.g. *N*-methyl; or (c) derivatives of the OH form, e.g. methyl ether. The placement of the derivatives within the DOC entry reflects these possibilities.

The policy for naming such compounds in DOC 6 is as follows:

1. All possible synonyms relating to both the NH and OH forms are given and can readily be found in the Name Index regardless of which tautomer is looked up.
2. The entry name for very simple compounds such as that shown above, for which the tautomerism is well studied, is the predominant tautomer, i.e. 2(1*H*)-Pyridinone.
3. In more complex cases where the tautomerism may or may not have been carefully investigated for individual members of the series, the hydroxyheteroaryl name is normally used as the entry name, with a note where appropriate indicating that the structure represented by the entry name may not be the predominant tautomer. This greatly simplifies the presentation of series of compounds (e.g. chlorodihydroxypyridines) where some are capable of NH tautomerism and some are not.

The same general principle is used for more complex cases where several different tautomers are present and where even 'blocked' derivatives such as *N*-methyl may still be capable of restricted tautomerism. For an example in DOC 6, see the series of naphthyridinediols.

The presentation of other types of tautomerism in DOC 6 follows the same general policy. In a few cases involving ring ⇌ chain tautomerism, the two tautomers have separate entries with cross-references between them.

2.2.3 Anions and cations

For ionic substances such as quaternary ammonium salts, the entry refers to the anion or cation and the molecular formula and molecular weight given are those of the ion. The various salts (e.g. chloride, nitrate) are treated as derivatives, each with its own molecular formula. Where a substance such as a dye is normally prepared and handled as, for example, a sodium salt, the entry usually refers to the parent acid.

2.3 Literature coverage

In compiling this edition the primary literature has been surveyed to mid-1994, and outstandingly important information from the second half of 1994 has been incorporated.

The first annual Supplement, which will appear in 1996, will survey the literature to mid-1995; thereafter annual Supplements will appear in the middle of each year and will be based on the literature to the middle of the previous calendar year. An even more topical coverage of the literature can be obtained from the CD-ROM version, which is republished complete on one disk every six months.

2.4 Organisation of entries

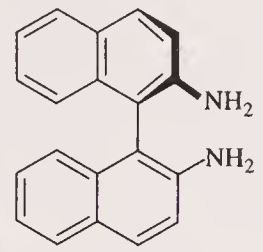
In general, the format of individual entries remains similar to that of previous editions. Figure 2.1 illustrates the format of a typical entry within which the individual types of data have been labelled. The range of information included within the entries is described below.

DOC name → **2,2′-Diamino-1,1′-binaphthyl** **D-0-00664** ← DOC Number

[1,1′-Binaphthalene]-2.2′-diamine, 9CI
2,2′-Diamino-1,1′-dinaphthyl
1,1′-Bi[2-naphthylamine]
} ← Alternative names (9CI, 8CI, other systematic, non-systematic)

CAS Registry Number → [4488-22-6]

Structural formula and stereochemical description →



(R)-form

← Molecular weight

$C_{20}H_{16}N_2$ M 284.360

← Use

Intermediate for chiral auxiliaries.

Molecular formula →

← Hazard description

Exp. tumorigen by skin contact. Dec. with emission of toxic fumes. DU3090000

← RTECS Number

Hazard alert symbol →

(R)-form [18741-85-0]
Mp 242.5–243. $[\alpha]_D^{21.4}$+ 155.5 (c, 1 in Py).
$[\alpha]_D^{18}$+ 46.8 (2*M* HCl).

Stereoisomer heading →

N,N′-*Di-Me*: [93713-30-5]
Cryst. (EtOH). Mp 143–144°.
$[\alpha]_D^{23}$+ 182 (c, 1.09 in C_6H_6).
} ← Physical data

Derivative subheading →

N,N,N′,N′-*Tetra-Me*: [135029-77-5]
Cryst. (EtOH/C_6H_6). Mp 216–218°.

(S)-form[18531-95-8]
Cryst. Mp 243° (235–239°).
$[\alpha]_D^{20}$– 149 (py). $[\alpha]_D^{19}$– 46 (2*M* HCl).

N,N′-*Di-Ac*:
$C_{24}H_{20}N_2O_2$ M 386.434
Prisms (C_6H_6). Mp 226–227°.
$[\alpha]_D^{25}$+ 10.8 (c, 1 in THF).

(±)-form [79082-81-8]
Silvery plates (EtOH). Mp 193.2–194.5° (191°).

Derivative subheading → *Picrate:*
Brownish-yellow plates (C_6H_6).
Mp 185° dec.

N,N′-*Di-Ac*:
Cubes (EtOH). Mp 235–236°.

N,N′-*Dibenzoyl*:
$C_{34}H_{24}N_2O_2$ M 492.576
Prisms ($PhNO_2$). Mp 235°.

[93621-61-5, 97644-73-0] ← Additional CAS Registry Numbers

Bibliographic references →

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Cumming, W.M. *et al, J.C.S.,* 1932, 528 (synth)
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Akimoto, H. *et al, Tetrahedron,* 1971, **27,** 5999 (resoln, abs config)
Miyano, S. *et al, Bull. Chem. Soc. Jpn.,* 1984, **57,** 2171 (pmr, ir, deriv)
Brown, K.J. *et al, J.O.C.,* 1985, **50,** 4345 (synth, resoln)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1989, **14,** 32 (use)
Smrčina, M. *et al, J.O.C.,* 1992, **57,** 1917 (synth, resoln, bibl)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials,* 8th Ed., Van Nostrand-Reinhold, 1992, BGB750

← Reference contents

Figure 2.1 The format of a typical entry in DOC 6, showing the individual types of data that may be included.

The *Dictionary of Organic Compounds* is also available as a database on CD-ROM. Entries may be displayed on screen or output in a format similar to that of the printed work. Powerful text retrieval and structure search software allows searches to be carried out not only on chemical names, molecular formulae and CAS Registry Number but also text words, hazard and toxicity information, labelled references, physical description and the physical properties using browsable indexes.

Structure and substructure searching using PsiBase for Windows™ rapidly allows the user to find all entries with particular structural features, and searches may be readily combined or refined.

The CD-ROM version of DOC 6 is available on subscription, which provides bi-annual updates in the form of a replacement CD-ROM containing updates and important new compounds from the chemical literature.

2.4.1 Chemical names and synonyms

(*a*) DOC Names

The DOC Name is that chosen to head each entry and is that which, in the opinion of the Editors, is most likely to be known by, and of use to, most readers. Systematic names following IUPAC conventions are used wherever feasible, but trivial names are used for most natural products, where systematic names are too cumbersome for convenient use. In cases where no one name stands out as being clearly more familiar or convenient than others, the *Chemical Abstracts* name is usually given precedence. In this edition, there has been some further revision of DOC nomenclature towards greater standardisation with CAS, especially for example in the choice of CAS Names such as '1,2-benzenediamine' as the entry names for aromatic and heterocyclic compounds in preference to the formerly preferred '1,2-diaminobenzene', etc.

The legislating body for chemical nomenclature is the International Union of Pure and Applied Chemistry (IUPAC). It is important to recognise that, while IUPAC lays down rules and principles for good nomenclature, application of those rules will not necessarily lead to a unique name for each compound. In other words, a compound may have more than one valid name conforming to IUPAC principles. Developments of IUPAC nomenclature, especially CAS nomenclature, introduce more rigid principles so as to arrive at a unique name for every possible compound.

It is important to emphasise this point, because it is a common misconception that the correct application of IUPAC rules will produce one, and one only, name for each compound, and therefore if a publication such as DOC presents two or more names, one of them must be 'wrong'. The situation is described in more detail in the preamble to the publication *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*, eds R. Panico *et al.* (Blackwell):

> It is important to recognize that the rules of systematic nomenclature need not necessarily lead to a unique name for each compound, but must always lead to an unambiguous one. Lucidity in communication often requires that the rules be applied with different priorities. A comparative discussion of the compounds CH_3–CH=CH_2, Cl–CH_2–CH=CH_2, C_6H_5–CH_2–CH=CH_2, H_2N–CH_2–CH=CH_2, and HO–CH_2–CH=CH_2, might be easier to follow if they were all named as propenes, even though with the last three, the benzene ring, amino, and hydroxy groups may have seniority over the double bond for citation as a parent or as a suffix. In other cases, a set of rules that generates clear and efficient names for some compounds can lead to clumsy and nearly unrecognizable names for others, even closely related ones. To force the naming of all compounds into the Procrustean bed of one set of rules would not serve the needs of general communication, and the Commission believes that the majority of organic chemists would not accept such a policy for general communication. This situation can be illustrated by a compound that most chemists would probably name as 'pentaphenylethane', instinctively, whereas the application of a principle favouring rings over chains leads to a name such as 'ethanepentaylpentabenzene'. The first name is certainly more easily recognized than the second ....
>
> In view of the foregoing considerations, this *Guide to IUPAC Nomenclature of Organic Compounds* often presents alternative sets of rules, equally systematic, wherever available and justifiable, to enable a user to fit the name to a particular need.
>
> Lastly, the Commission recognizes that for certain types of compounds, there is significant disagreement among chemists in different fields as to what should be the preferred nomenclature. This situation leads to an apparent lack of decisiveness in some of the recommendations in this document. This is unavoidable, because long experience has taught that formulating rules not having general support is a futile exercise; such rules will be widely ignored. Therefore, the Commission's policy is to offer critically examined alternatives, some of which may be new proposals, and to observe how they are accepted and used. If one of the alter-

natives subsequently becomes preferred to an overwhelming extent by the community of chemists, a future edition of recommentations can reflect that fact.

In this Guide, some practices of the Chemical Abstracts Service and/or of the Beilstein Institute have been mentioned. This is done only for informational purposes, and such instances are not necessarily recommendations of the Commission. The Commission recognized that there are circumstances that require a preferred (i.e. unique) name. These include comprehensive indexing (such as for the volume indexes to *Chemical Abstracts*) in order to avoid an intolerable amount of cross-indexing and multiple entries. This need is being met in a particular way by Chemical Abstracts Service as in-house procedures designed to place compounds with the same parent skeleton together while at the same time minimizing the number of rules. The *Chemical Abstracts Index Guide* treats the majority of compounds, but is not complete. There are a number of other in-house procedures applied elsewhere, such as in *Beilstein* (not yet explicitly published).

(*b*) Synonyms

An important function of DOC is to present a wide range of synonyms. In general the selection is made as useful as possible, but no attempt is made to provide exhaustive lists of proprietary names for pharmaceuticals and other commercially available compounds.

Editorial policy on minor points of nomenclature is as follows:

- Propanoic vs propionic and butanoic vs butyric; the former are preferred, particularly in entry names.
- Sulfur vs sulphur; the former is used.
- *Chemical Abstracts* practice regarding the position of locant numerals is generally followed; e.g. 2-hepten-1-ol is preferred to hept-2-en-1-ol.
- Eicosa vs icosa and oestr vs estr; the former are given priority but the alternative spellings are given as synonyms and thus appear in the Name Index.

The editorial generation of new synonyms that are not in the literature has been kept to a minimum.

CA names

Names corresponding to those used by Chemical Abstracts Service during the Eighth and Ninth Collective Index periods (1967–71 and 1972–76 respectively) are labelled with the suffixes 8CI and 9CI respectively. It should be noted that 9CI nomenclature is defined as that brought into use by CAS at the beginning of the Ninth Collective Index period, and that for organic compounds has been carried over essentially unchanged into subsequent Collective Index periods. Therefore the suffix '9CI' does *not* mean that the compound can necessarily be found in the Ninth Collective Index, as it may have been indexed only since 1976.

Recommended names

Names recommended by various regulatory bodies and standards associations are given suffixes to denote their origin:

ANSI	American National Standards Institute
BAN	British Approved Name
BSI	British Standards Institution
INN	International Nonproprietary Name
ISO	International Standards Organisation
JAN	Japanese Accepted Name
USAN	United States Adopted Name
WSSA	Weed Science Society of America

Note that no distinction is made between proposed and recommended INNs.

2.4.2 CAS Registry Numbers

CAS Registry Numbers have been included for as many compounds as possible. For a description of CAS Registry Numbers, see Chapter 10. While every attempt has been made to achieve *accuracy* of the reported Registry Numbers, no guarantee can be provided as to the *comprehensiveness* of the range of numbers presented. Thus, the absence of a Registry Number does not necessarily imply that one has not been allocated.

Registry Numbers that clearly belong to an entry but which cannot be unequivocally matched up to any of the individual compounds covered by that entry are given at the end of the entry. These additional Registry Numbers fall into one of the following categories:

- Duplicate Registry Numbers.
- Registry Numbers assigned to trivial variants of a compound, e.g. hydrates.
- Registry Numbers of stereoisomers or derivatives for which no physical data can readily be found.
- Registry Numbers referring to entities that are not specifically treated by the DOC entry.

- Registry Numbers referring to non-specific isomers.

For further information about CAS Registry Numbers, see Chapter 10.

2.4.3 Structural formulae

The structures in DOC are drawn as accurately as possible according to best current practice and IUPAC recommendations. In drawing the formulae, as much consistency as possible between closely related structures has been aimed at. Thus, for example, sugars have been standardised as Haworth formulae and wherever possible in complex structures the rings are orientated in the standard Haworth manner so that structural comparisons can quickly be made.

In a series of closely related compounds, e.g. a series of aromatic or heteroaromatic isomers, the structural formula is given only for the first member.

2.4.4 Stereochemical conventions

Where the absolute configuration of a compound is known or can be inferred from the published literature without undue difficulty, this is indicated. Where only one stereoisomer is referred to in the text, the structural diagram indicates that stereoisomer.

Various methods of describing stereochemistry are used (these are described elsewhere in this volume):

- The (*R*,*R*)-system for chiral molecules (see Section 8.2, under *R*-).
- The D,L-system for sugars and amino acids (see Section 8.2, under D-).
- The α,β-system for complex natural products such as steroids, for other cyclic molecules and for anomers of sugars (see Section 8.2, under *steroids*).
- The (*E*,*Z*)-system for specifying configurations at double bonds (see Section 8.2, under *E*-).
- The *ent*-convention where there is configurational inversion at all of the chiral centres whose configuration is implied in a name (see Section 8.2, under *ent*-).
- The *sn*-convention for glycerides (see Section 8.2, under *sn*-).

2.4.5 Molecular formula and molecular weight

The elements in the molecular formula are given according to the Hill convention (C, H, then other elements in alphabetical order). The molecular weights given are formula weights (or, more strictly, molar masses in daltons) and are computer calculated from the most current IUPAC table of atomic weights and rounded to three decimal places. In the case of some high-molecular-mass substances such as proteins, the value quoted may be that taken from an original literature source and may be an aggregate molar mass.

2.4.6 Importance/use

Care has been taken in DOC to make the information given on the importance and uses of chemical substances as accurate as possible. Wherever possible, information on a particular use has been checked against a critical source, such as the *Kirk-Othmer Encyclopedia of Chemical Technology* or *Ullmann's Encyclopedia of Industrial Chemistry*.

2.4.7 Physical data

(*a*) Melting points and boiling points

Melting and boiling points are reported in degrees Celsius. The policy followed in the case of conflicting data is as follows:

- Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted.
- Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure), the lower figure is given in parentheses; thus 139° (135–136°).
- Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses; thus 142°, 205–206°.
- Known cases of polymorphism or double melting point are noted.
- Boiling points are given at atmospheric pressure unless otherwise indicated. The pressure in mmHg (if not atmospheric) is given as a subscript, e.g.

Bp_{100} 85°. Some boiling points are now quoted in the literature with the pressure given using the SI unit kPa (kilopascals); for the time being, DOC retains mmHg. The conversion factor is: 1 mmHg = 0.133 222 kPa; 1 kPa = 7.500 64 mmHg.

(*b*) Optical rotations

Optical rotations are given wherever possible. They are expressed in the form: $[\alpha]_D^{20}$ +30.6 (c, 1.2 in $CHCl_3$). This denotes a temperature of 20 °C, wavelength at the sodium D line (589 nm) and a concentration of 1.2 g/100 ml in chloroform solution. In many cases, an indication of optical purity (op) or enantiomeric excess (ee) is reported after the value, if it is given in the literature. The degree sign formerly given following optical rotations, and which is still extensively found in the primary literature, has been dropped as it is dimensionally incorrect.

(*c*) Densities and refractive indices

Densities and refractive indices are now of less importance for the identification of liquids than has been the case in the past, but are still quoted for relatively common substances such as solvents. Many literature values for refractive indices are based on relatively impure samples obtained before modern purification methods were available. This applies particularly to natural products such as monoterpenes. Densities and refractive indices are not quoted where the determination appears to refer to undefined mixtures of stereoisomers.

(*d*) Solubilities

Solubilities are given only where the solubility is unusual for an organic compound. Most organic compounds not containing polar groups are soluble in typical organic solvents, e.g. ether, and insoluble in water.

(*e*) pK_a values

pK_a values are given for both acids and bases. The pK_a of a base can be obtained by subtracting its pK_b from 14.17 (at 20 °C) or from 14.00 (at 25 °C).

(*f*) Spectroscopic data

Spectroscopic data, such as uv wavelengths and extinction coefficients, are given where the spectrum is a main point of interest, or where the compound is unstable and has been identified only by spectroscopic data. In many other cases, spectroscopic data can be located through the references quoted. Spectroscopic data (initially uv and cmr) are now being introduced into the CD-ROM versions in a form that makes the data both numerically searchable and displayable on-screen.

2.4.8 Toxicity and hazard information

(*a*) General

An important function of a DOC 6 entry is to alert the user to potential hazards associated with the use of the compound. This information is highlighted by the sign ▷ (which also appears in the indexes). For this edition of DOC, all hazard and toxicity data have been carefully and critically assessed, and re-edited by a specialist Editor. Brief summaries of hazard and toxicity information have been included with the data for many chemical substances, particularly where there have been reports of adverse effects in people or where an incident in a laboratory has revealed the reactive nature of a chemical. As with the RTECS Accession Numbers, the sign ▶ is used to highlight summaries of hazard and toxicity data. Any references to this information in the primary literature or the standard monographs that have been quoted in this edition will usually carry the tags (*haz*) or (*tox*). A more detailed explanation of the choice of hazard and toxicity information for DOC may be found in Chapter 12.

Although much care has been taken to ensure the accuracy and completeness of reported data, *DOC must not be considered a comprehensive source on hazard data*. The function of hazard data in DOC 6 is to alert the user to possible hazards associated with the use of a particular compound, but the absence of such data cannot be taken as an indication of safety in use, and the publishers cannot be held responsible for any inaccuracies in the reported information.

Further details of DOC coverage of toxicity and hazard information can be found in Chapter 12.

(*b*) RTECS Accession Numbers

Many entries in DOC 6 contain one or more RTECS Accession Numbers. These numbers refer to toxicity information on the relevant compounds from the

NIOSH Registry of Toxic Effects of Chemical Substances.

The *Registry* is a compendium of toxicity data extracted from the scientific literature. A CD-ROM version of RTECS is updated quarterly and is most conveniently searched using the RTECS Accession Number or CAS Number given in DOC.

For each RTECS Accession Number the RTECS database provides the following data where available: substance prime name and synonyms; date when the substance record was last updated; CAS Registry Number; molecular weight and formula; reproductive, tumorigenic and toxic dose data; and citations to aquatic toxicity ratings, IARC reviews, ACGIH Threshold Limit Values, toxicological reviews, existing Federal standards, the NIOSH criteria document programme for recommended standards, the NIOSH current intelligence programme, the NCI Carcinogenesis Testing Program, and the EPA Toxic Substances Control Act inventory. Each data line and citation is referenced to the source from which the information was extracted.

2.4.9 Bibliographic references

The selection of references in DOC is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. In general, recent references are preferred to older ones. The number of references quoted cannot be taken as an indication of the relative importance of a compound, since, where a good modern reference is available that contains an accurate bibliography of previous work on the compound, this reference may be cited in place of several older ones. Such references often carry the reference tags (*bibl*) or (*rev*). For very common compounds that are nowadays readily available in quantity, long lists of preparations are not presented but the emphasis is on references to spectra, chromatography, etc.

(*a*) Suffixes

The content of many references is indicated by means of suffixes, of which the following are the most important:

(abs config)	absolute configuration
(anal)	analysis
(bibl)	bibliography
(cd)	circular dichroism
(chromatog)	chromatography
(cmr)	carbon (^{13}C) nuclear magnetic resonance
(conformn)	conformation
(cryst struct)	X-ray crystal structure determination
(deriv)	reference referring to a derivative
(epr)	electron paramagnetic resonance (also called electron spin resonance, esr)
(glc)	gas–liquid chromatography
(haz)	hazard
(hplc)	high-performance liquid chromatography
(ir)	infrared spectrum
(isol)	isolation
(isom)	isomerism
(manuf)	manufacture
(metab)	metabolism
(ms)	mass spectrum
(nmr)	nuclear magnetic resonance (general)
(occur)	occurrence
(ord)	optical rotatory dispersion
(pharmacol)	pharmacology
(pmr)	proton (^{1}H) nuclear magnetic resonance
(polarog)	polarography
(props)	properties (chemical or physical)
(resoln)	resolution
(rev)	review
(synth)	synthesis
(tautom)	tautomerism
(tox)	toxicity
(uv)	ultraviolet or visible spectrum

Some recently added references carry the tag **synth** in bold type. This is used to highlight a synthesis that is claimed by the authors to be a clear improvement on existing methods (e.g. in yield, simplicity of procedure, avoidance of toxic starting materials, etc.) and in which full experimental details are given.

Some items of information, particularly the physical properties of derivatives of long-known compounds, may arise from references not cited in this edition.

(*b*) Journal abbreviations

For the journals in the following list, the abbreviations shown are used in DOC 6. For all other journals,

the practice of the *Chemical Abstracts Service Source Index* (CASSI) is followed.

Fuller abbreviated title	Shortened title used in DOC 6
Acta Crystallogr.	*Acta Cryst.*
Acta Crystallogr., Sect. A	*Acta Cryst. A*
Acta Crystallogr., Sect. B	*Acta Cryst. B*
Acta Crystallogr., Sect. C	*Acta Cryst. C*
Acta Crystallogr. (Suppl.)	*Acta Cryst. (Suppl.)*
Angew. Chem., Int. Ed. Engl.	*Angew. Chem., Int. Ed.*
Collect. Czech. Chem. Commun.	*Coll. Czech. Chem. Comm.*
J. Am. Chem. Soc.	*J.A.C.S.*
J. Chem. Soc.	*J.C.S.*
J. Chem. Soc. A	*J.C.S.(A)*
J. Chem. Soc. B	*J.C.S.(B)*
J. Chem. Soc. C	*J.C.S.(C)*
J. Chem. Soc., Chem. Commun.	*Chem. Comm.*
J. Chem. Soc., Dalton Trans.	*J.C.S. Dalton*
J. Chem. Soc., Faraday Trans. 1	*J.C.S. Faraday 1*
J. Chem. Soc., Faraday Trans. 2	*J.C.S. Faraday 2*
J. Chem. Soc., Perkin Trans. 1	*J.C.S. Perkin 1*
J. Chem. Soc., Perkin Trans. 2	*J.C.S. Perkin 2*
J. Heterocycl. Chem.	*J. Het. Chem.*
J. Nat. Prod. (Lloydia)	*J. Nat. Prod.*
J. Org. Chem.	*J.O.C.*
Justus Liebigs Ann. Chem.	*Annalen*
Recl. Trav. Chim. Pays-Bas (J.R. Neth. Chem. Soc.)	*Rec. Trav. Chim. (J.R. Neth. Chem. Soc.)*
Spectrochim. Acta, Part A	*Spectrochim. Acta A*
Spectrochim. Acta, Part B	*Spectrochim. Acta B*
Tetrahedron Lett.	*Tet. Lett.*

On the whole, patents are not cited where the equivalent information is available from a journal citation. No distinction is made between patent applications and granted patents.

2.5 Abbreviations used in DOC

[α]	specific rotation
abs. config.	absolute configuration
Ac	acetyl
ACGIH	threshold limit values from the American Conference of Governmental Industrial Hygienists
Ac_2O	acetic anhydride
AcOH	acetic acid
alk.	alkaline
amorph.	amorphous
anal.	analytical applications, analysis or detection
anhyd.	anhydrous
approx.	approximately
aq.	aqueous
asym.	asymmetrical
BAN	British Approved Name
bibl.	bibliography
biol.	biological
biosynth.	biosynthesis
Bp	boiling point
c.	concentration
ca.	(circa) about
cd	circular dichroism
chromatog.	chromatography
cmr	^{13}C nuclear magnetic resonance spectrum
col.	colour, coloration
comly.	commercially
compd(s).	compound(s)
conc.	concentrated
config.	configuration
conformn.	conformation
constit.	constituent
d.	density
dec.	decomposes, decomposition
deg.	degree
deriv(s)	derivative(s)
descr.	described
detn.	detection/determination
dil.	dilute, dilution
dimorph.	dimorphic
diss.	dissolves, dissolved
dissoc.	dissociates
dist.	distil, distillation
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
ee	enantiomeric excess
electrochem.	electrochemistry, electrochemical
epr	electron paramagnetic resonance spectrum
eq.	equivalent

equilib.	equilibrium
esp.	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
EtOH aq.	aqueous ethanol
evapn.	evaporation
exp.	experimental
fl.p.	flash point
fluor.	fluoresces, fluorescence
formn.	formation
Fp	freezing point
glc	gas–liquid chromatography
h	hour
haz.	hazard
hplc	high-performance liquid chromatography
hydrol.	hydrolyses, hydrolysed, hydrolysis
hν	light
INN	International Nonproprietary Name
insol.	insoluble
intermed.	intermediate
ir	infrared spectrum
isol.	isolated
isom.	isomerises
JAN	Japanese Accepted Name
LD	lethal dose
LD_{50}	a calculated dose that is expected to cause the death of 50% of an entire animal population
manuf.	manufacturer, manufactured
max.	maximum
Me	methyl
MeCN	acetonitrile
Me_2CO	acetone
MeOH	methanol
metab.	metabolite, metabolism
misc.	miscible/miscellaneous
mixt.	mixture
mod.	moderately
mol	mole
Mp	melting point
ms	mass spectrum
n	index of refraction, e.g. n_D^{20} for 20°C and sodium light
nmr	nuclear magnetic resonance spectrum
obt.	obtained
occur.	occurrence
OES	occupational exposure standards (British)
op	optical purity
ord	optical rotatory dispersion
org.	organic
Ph	phenyl (C_6H_5)
pharmacol.	pharmacology
phys.	physical
pmr	proton magnetic resonance spectrum
polarog.	polarography
polym.	polymerised, polymerisation
prob.	probably
prop(s).	property (properties)
purifn.	purification
Py	pyridine
ref.	reference
rel.	relative(ly)
resoln.	resolution
rev.	review
r.t.	room temperature
sepn.	separation
sl.	slightly
sol.	soluble
soln(s).	solution(s)
solv(s).	solvent(s)
sp.	species (singular)
spar.	sparingly
spp.	species (plural)
ssp.	subspecies
subl.	sublimation, sublimes
synth.	synthesis
tautom.	tautomerism
temp(s)	temperature(s)
THF	tetrahydrofuran
tlc	thin-layer chromatography
TLV	Threshold Limit Value
tox.	toxicity/toxicology
unsatd.	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
v.	very
var.	variety
vis.	visible
vol.	volume
Vp	vapour pressure

3 Organic chemistry journals

This list gives details of the principal journals in organic chemistry plus some of the more important journals in inorganic chemistry and biochemistry.

The following items of information are given:

- Full journal titles.
- CASSI abbreviated titles. CASSI (the *Chemical Abstracts Service Source Index*) includes details on all journals cited in *Chemical Abstracts* since 1907 together with some cited in *Beilstein* and *Chemisches Zentralblatt* as far back as 1830. CASSI gives an abbreviated title for each journal; these abbreviated titles, which are based on internationally recognised systems, are used for citing references in many publications.
- The abbreviated form of journal title that appears in DOC 6, if different from the CASSI abbreviated title (this applies to a few common journals only).
- Years of publication.
- CODENs for titles published since ca. 1965. A CODEN is a six-character code that uniquely identifies a publication. Each journal title has its own CODEN, and they are especially useful in online searching.
- A statement that a journal does not have volume numbers; details of when volume numbers were discontinued (e.g. *Liebigs Ann. Chem., J. Chem. Soc.*) or introduced (e.g. *Tetrahedron Lett., Bull. Soc. Chim. Fr.*); series of volume numbers (e.g. *Ann. Chim. (Paris)*).
- Some indication of subject matter (where not obvious from the title), especially for those titles issued as two or more parts (e.g. *An. Quim., J. Chem. Soc.*).
- Changes of title and superseded titles.
- Translation journals.
- Any other useful information.

Accounts of Chemical Research [*Acc. Chem. Res.*] (1968–; ACHRE4). Review journal

ACS Symposium Series [*ACS Symp. Ser.*] (1974–; ACSMC8). Irregular

Acta Chemica Scandinavica [*Acta Chem. Scand.*] (1947–73; ACSAA4; 1989–; ACHSE7). From 1974–88 (vols 29–42) divided into: Series A [*Acta Chem. Scand., Ser. A*] (ACAPCT) (physical and inorganic chemistry); and Series B [*Acta Chem. Scand., Ser. B*] (ACBOBV) (organic chemistry and biochemistry)

Acta Chimica Hungarica [*Acta Chim. Hung.*] (1983–; ACHUDC). Formerly *Hungarica Acta Chimica* [*Hung. Acta Chim.*] (1946–49) and *Acta Chimica Academiae Scientiarum Hungaricae* [*Acta Chim. Acad. Sci. Hung.*] (1951–82; ACASA2)

Acta Chimica Sinica see *Huaxue Xuebao*

Acta Crystallographica [*Acta Crystallogr.*; *Acta Cryst.* in DOC 6] (1948–67; ACCRA9). In 1968, divided into: Section A [*Acta Crystallogr., Sect. A*; *Acta Cryst. A* in DOC 6] (1968–; ACACBN, ACACEQ) (fundamentals of crystallography); and Section B [*Acta Crystallogr., Sect. B*; *Acta Cryst. B* in DOC 6] (1968–; ACBCAR) (structural sciences). Later sections to be added are: Section C [*Acta Crystallogr., Sect. C*; *Acta Cryst. C* in DOC 6] (1983–; ACSCEE) (crystal structure communications), formerly *Crystal Structure Communications* [*Cryst. Struct. Commun.*] (1972–82; CSCMCS); and Section D [*Acta Crystallogr., Sect. D*; *Acta Cryst. D* in DOC 6] (1993–; ABCRE6) (biological crystallography)

Acta Pharmaceutica [*Acta Pharm. (Zagreb)*] (1992–; ACPHEE). Formerly *Acta Pharmaceutica Jugoslavia* [*Acta Pharm. Jugoslav.*] (1951–91; APJUA8)

Acta Pharmaceutica Fennica see *European Journal of Pharmaceutical Sciences*

Acta Pharmaceutica Nordica see *European Journal of Pharmaceutical Sciences*

Acta Pharmaceutica Suecica see *European Journal of Pharmaceutical Sciences*

Advances in Chemistry Series [*Adv. Chem. Ser.*] (1950–; ADCSAJ). Irregular

Agricultural and Biological Chemistry see *Bioscience, Biotechnology, and Biochemistry*

Aldrichimica Acta [*Aldrichim. Acta*] (1968–; ALACBI)

American Chemical Journal see *Journal of the American Chemical Society*

Anales de Quimica [*An. Quim.*] (1968–79; ANQUBU; 1990–; ANQUEX). From 1980–89, divided into: Series A [*An. Quim., Ser. A*] (AQSTDQ) (physical and technical); Series B [*An. Quim., Ser. B*] (AQSAD3) (inorganic and analytical); and Series C [*An. Quim., Ser. C*] (AQSBD6) (organic and biochemical)

Angewandte Chemie [*Angew. Chem.*] (1988–; ANCEAD). From 1888–1941, the title was *Zeitschrift für Angewandte Chemie* [*Z. Angew. Chem.*]. In German, but in 1962 an International Edition in English [*Angew. Chem. Int. Ed. Engl.*; *Angew. Chem. Int. Ed.* in DOC 6] (1962–; ACIEAY) was launched. The German and English editions have different volume and page numbers. Vol. 1 of the International edition corresponds to vol. 74 of the German edition. In 1982 and 1983, miniprint supplements were issued. In 1991, *Angewandte Chemie* absorbed *Zeitschrift für Chemie* [*Z. Chem.*] (1961–90; ZECEAL)

Annalen see *Liebigs Annalen*

Annalen der Chemie und Pharmazie see *Liebigs Annalen*

Annales de Chimie [*Ann. Chim. (Paris)*] (1789–; ANCPAC). From 1816–1913, the title was *Annales de Chimie et de Physique* [*Ann. Chim. Phys.*]. There have been various series of volume numbers: the 15th series, vol. 1 appeared in 1976. Since 1973 this journal has specialised in solid-state chemistry; in 1978 *Science de Materiaux* became a subtitle

Annales Pharmaceutiques Français [*Ann. Pharm. Fr.*] (1943–; APFRAD). Formed by a merger of *Journal de Pharmacie et de Chemie* [*J. Pharm. Chim.*] (1842–1942) and *Bulletin des Sciences Pharmacologiques* [*Bull. Sci. Pharmacol.*] (1899–1942)

Annali di Chimica [*Ann. Chim. (Rome)*] (1950–; ANCRAI). Formerly *Annali di Chimica Applicata* [*Ann. Chim. Appl.*] (1941–49)

Annals of the New York Academy of Science [*Ann. N.Y. Acad. Sci.*] (1877–; ANYAA9). Irregular. No issue numbers

Antibiotiki i Khimioterapiya [*Antibiot. Khimioter.*] (1988–; ANKHEW). Formerly *Antibiotiki* [*Antibiotiki (Moscow)*] (1956–84; ANTBAL) and *Antibiotiki i Meditsinskaya Bioteknologiya* [*Antibiot. Med. Biotekhnol.*] (1985–87; ANBIEH)

Applied Organometallic Chemistry [*Appl. Organomet. Chem.*] (1987–; AOCHEX)

Archiv der Pharmazie [*Arch. Pharm. (Weinheim, Ger.)*] (1835–; APRMAS). From 1924–71 known as *Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft* [*Arch. Pharm. Ber. Dtsch. Pharm. Ges.*]

Archives of Biochemistry and Biophysics [*Arch. Biochem. Biophys.*] (1951–; ABBIA4). Formerly *Archives of Biochemistry* [*Arch. Biochem.*] (1942–51)

Arhiv za Kemiju see *Croatica Chemica Acta*

Arkiv for Kemi see *Chemica Scripta*

Arzneimittel-Forschung [*Arzneim.-Forsch.*] (1951–; ARZNAD). Drug research

Australian Journal of Chemistry [*Aust. J. Chem.*] (1953–; AJCHAS). Superseded *Australian Journal of Scientific Research, Series A* [*Aust. J. Sci. Res., Ser. A*] (1948–52)

Berichte see *Chemische Berichte*

Berichte der Deutschen Chemischen Gesellschaft see *Chemische Berichte*

Biochemical and Biophysical Research Communications {*Biochem. Biophys. Res. Commun.*] (1959–; BBRCA9)

Biochemical Journal [*Biochem. J.*] (1906–; BIJOAK). Beginning in 1973 alternate issues are subtitled *Molecular Aspects* and *Cellular Aspects*

Biochemical Society Transactions [*Biochem. Soc. Trans.*] (1973–; BCSTB5). Replaced a proceedings section formerly included in *Biochemical Journal*

Biochemistry [*Biochemistry*] (1962–; BICHAW)

Biochemistry and Molecular Biology International [*Biochem. Mol. Biol. Int.*] (1993–; BMBIES). Formerly *Biochemistry International* [*Biochem. Int.*] (1980–; BIINDF)

Biochemistry International see *Biochemistry and Molecular Biology International*

Biochimica Biophysica Acta [*Biochim. Biophys. Acta*] (1947–; BBACAQ)

Biochimie [*Biochimie*] (1971–; BICMBE). Formerly *Bulletin de la Société de Chimie Biologique* [*Bull. Soc. Chim. Biol.*] (1914–70; BSCIA3)

Biological and Pharmaceutical Bulletin see *Chemical and Pharmaceutical Bulletin*

Biological Chemistry Hoppe-Seyler [*Biol. Chem. Hoppe-Seyler*] (1985–; BCHSEI). Formerly *Zeitschrift für Physiologische Chemie* [*Z. Physiol. Chem.*] (1877–1895) and *Hoppe-Seylers Zeitschrift für Physiologische Chemie* [*Hoppe-Seylers Z. Physiol. Chem.*] (1895–1984; HSZPAZ)

Biological Mass Spectrometry see *Journal of Mass Spectrometry*

Biomedical and Environmental Mass Spectrometry see *Journal of Mass Spectrometry*

Biomedical Mass Spectrometry see *Journal of Mass Spectrometry*

Bioorganic and Medicinal Chemistry [*Bioorg. Med. Chem.*] (1993–; BMECEP)

Bioorganic and Medicinal Chemistry Letters [*Bioorg. Med. Chem. Lett.*] (1991–; BMCLE8)

Bioorganic Chemistry [*Bioorg. Chem.*] (1971–; BOCMBM)

Bioorganicheskaia Khimia [*Bioorg. Khim.*] (1975–; BIKHD7). In Russian. There is an English translation called *Soviet Journal of Bioorganic Chemistry* [*Sov. J. Bioorg. Chem. (Engl. Transl.)*] (1975–; SJBCD5)

Bioscience, Biotechnology, and Biochemistry [*Biosci., Biotechnol., Biochem.*] (vol. 56; 1992–; BBBIEJ). Formerly *Bulletin of the Agricultural Chemical Society of Japan* [*Bull. Agric. Chem. Soc. Jpn.*] (1924–60); and *Agricultural and Biological Chemistry* [*Agric. Biol. Chem.*] (1961–91; ABCHA6)

Bulletin de la Société de Chimie Biologique see *Biochimie*

Bulletin de la Société Chimique de France [*Bull. Soc. Chim. Fr.*] (1858–; BSCFAS). No volume numbers between 1955 and 1991; 1992 is vol. 129. For several years each issue was split into two parts with Partie II containing the items on organic chemistry. From 1978–84, the two parts each had parallel page numbering; in order to distinguish between the two parts, the page numbers were prefixed by the part number, e.g. II-579

Bulletin des Sciences Pharmacologiques see *Annales Pharmaceutiques Français*

Bulletin des Sociétés Chimique Belges [*Bull. Soc. Chim. Belg.*] (1904–; BSCBAG)

Bulletin of the Academy of Sciences of the USSR, Division of Chemical Sciences see *Izvestiya Akademii Nauk, Seriya Khimicheskaya*

Bulletin of the Chemical Society of Japan [*Bull. Chem. Soc. Jpn.*] (1926–; BCSJA8)

Bulletin of the Polish Academy of Sciences, Chemistry [*Bull. Pol. Acad. Sci., Chem.*] (1983–; BPACEQ). Formerly *Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques* [*Bull. Acad. Pol. Sci., Ser. Sci. Chim.*] (1960–82; BAPCAQ).

Bulletin of the Research Council of Israel see *Israel Journal of Chemistry*

Canadian Journal of Chemistry [*Can. J. Chem.*] (1951–; CJCHAG). Continuation of Canadian Journal of Research [*Can. J. Res.*] (1929–35) and its subsequent Section B [*Can. J. Res., Sect. B*] (1935–50) (chemical sciences)

Carbohydrate Research [*Carbohydr. Res.*] (1965–; CRBRAT)

Chemical and Pharmaceutical Bulletin [*Chem. Pharm. Bull.*] (1958–; CPBTAL). Formerly *Pharmaceutical Bulletin* [*Pharm. Bull.*] (1953–57). In 1993 biologically oriented papers were transferred to *Biological and Pharmaceutical Bulletin* [*Biol. Pharm. Bull.*] (1993–; BPBLEO)

Chemical Communications [*Chem. Comm.*] (1965–69; CCOMA8) became part D [*J. Chem. Soc. D*] (1970–71)

Chemical Papers [*Chem. Pap.*] (1985–; CHPAEG). Formerly *Chemicke Zvesti* [*Chem. Zvesti*] (1947–84; CHZVAN)

Chemical Reviews [*Chem. Rev.*] (1924–; CHREAY)

Chemical Society Reviews [*Chem. Soc. Rev.*] (1972–; CSRVBR). Successor to *Quarterly Reviews of the Chemical Society* [*Q. Rev. Chem. Soc.*] (1947–71; QUREA7) and *RIC Reviews* [*RIC Rev.*] (1968–71; RREVBI)

Chemica Scripta [*Chem. Scr.*] (1971–89; CSRPB9). Successor to *Arkiv for Kemi* [*Ark. Kemi*] (1949–71; ARKEAD). No longer published

Chemicke Zvesti see *Chemical Papers*

Chemiker-Zeitung see *Journal für Praktische Chemie – Chemiker-Zeitung*

Chemische Berichte [*Chem. Ber.*] (1947–; CHBEAM). Formerly *Berichte der Deutschen Chemischen Gesellschaft* [*Ber. Dtsch. Chem. Ges.*] (1868–1945), which from 1919–45 was divided into Abteilung A [*Ber. Dtsch. Chem. Ges. A*] (Vereinsnachrichten) and Abteilung B [*Ber. Dtsch. Chem. Ges. B*] (Abhandlungen). Early volumes are often cited as *Berichte* [*Ber.*]. From 1995 accepts papers in English covering inorganic and organometallic chemistry only

Chemistry and Industry [*Chem. Ind. (London)*] (1923–; CHINAG). Until 1950, the title was *Journal of the Society of Chemical Industry: Chemistry and Industry* [*J. Soc. Chem. Ind.: Chem. Ind.*]. No volume numbers

Chemistry and Physics of Lipids [*Chem. Phys. Lipids*] (1966–; CPLIA4)

Chemistry Express [*Chem. Express*] (1986–93; CHEXEU) (Journal of Kinki Chemical Society, Japan). No longer published

Chemistry Letters [*Chem. Lett.*] (1972–; CMLTAG). No volume numbers

Chemistry of Heterocyclic Compounds see *Khimiya Geterotsiklicheskikh Soedinenii*

Chemistry of Natural Compounds see *Khimiya Prirodnykh Soedinenii*

Chimia [*Chimia*] (1947–; CHIMAD). No volume numbers

Chimica Therapeutica see *European Journal of Medicinal Chemistry*

Chinese Chemical Letters [*Chin. Chem. Lett.*] (1991–; CCLEE7)

Chinese Journal of Chemistry see *Huaxue Xuebao*

Collection of Czechoslovak Chemical Communications [*Collect. Czech. Chem. Commun.; Coll. Czech. Chem. Comm.* in DOC 6] (1929–; CCCCAK)

Comptes Rendus Hebdomadaires des Séances de l'Académie des Sciences [*C. R. Hebd. Seances Acad. Sci.*] (1835–1965; COREAF). In 1966, divided into: Series A [*C. R. Hebd. Seances Acad. Sci. Ser. A*] (1966–80; CHASAP) (mathematical sciences); Series B [*C. R. Hebd. Seances Acad. Sci. Ser. B*] (1966–80; CHDBAN) (physical sciences); Series C [*C. R. Hebd. Seances Acad. Sci. Ser. C*] (1966–80; CHDCAQ) (chemical sciences); and Series D [*C. R. Hebd. Seances Acad. Sci. Ser. D*] (1966–80; CHDDAT) (life sciences). Series A–D were superseded by: Series I [*C. R. Hebd. Seances Acad. Sci. Ser. 1*] (mathematics; formerly Series A) (1981–); Series II [*C. R. Hebd. Seances Acad. Sci. Ser. 2*] (physics, chemistry, astronomy, earth and planetary sciences; formerly Series B + C) (1981–; CRSUDO); and Series III [*C. R. Hebd. Seances Acad. Sci. Ser. 3*] (life sciences; formerly series D) (1981–; CRSEDA). Since 1984 (vol. 299), Sections I–III have been titled *Comptes Rendus de l'Académie des Sciences* [e.g. *C. R. Acad. Sci. Ser 1*]

Contemporary Organic Synthesis [*Contemp. Org. Synth.*] (1994–; COGSE6). Review journal

Croatica Chemica Acta [*Croat. Chem. Acta*] (1956–; CCACAA). Formerly *Arhiv za Kemiju* [*Arh. Kem.*] (1927–55)

Crystal Structure Communications see *Acta Crystallographia*

Doklady Akademii Nauk [*Dokl. Akad. Nauk*] (1933–; DAKNEQ). In Russian. Until 1992, the title was *Doklady Akademii Nauk SSSR* [*Dokl. Akad. Nauk SSSR*] (DANKAS). There is an English translation of the chemistry section called *Doklady Chemistry* [*Dokl. Chem. (Engl. Transl.)*] (1956–; DKCHAY)

Egyptian Journal of Chemistry [*Egypt. J. Chem.*] (1958–; EGJCA3). From 1960–69, the title was *Journal of Chemistry of the United Arab Republic* [*J. Chem. U.A.R.*] (JUARAK). From 1970–71, the title was *United Arab Republic Journal of Chemistry* [*U.A.R. J. Chem.*] (UAJCA2)

European Journal of Medicinal Chemistry [*Eur. J. Med. Chem.*] (1974–; EJMCA5). Formerly *Chimica Therapeutica* [*Chim. Ther.*] (1965–73; CHTPBA)

European Journal of Pharmaceutical Sciences [*Eur. J. Pharm. Sci.*] (1993–; EPSCED). Formed by a merger of *Acta Pharmaceutica Fennica* [*Acta Pharm. Fennica*] (1977–92; APHFDO) with *Acta Pharmaceutica Nordica* [*Acta Pharm. Nord.*] (1989–92; APNOEE). *Acta Pharmaceutica Nordica* was formed by a merger of: *Acta Pharmaceutica Suecica* [*Acta Pharm. Suec.*] (1964–88; APSXAS) and *Norvegica Pharmaceutica Acta* [*Norv. Pharm. Acta*] (1983–86; NPACDL)

Experientia [*Experientia*] (1945–; EXPEAM)

Farmaco [*Farmaco*] (1989–; FRMCE8) (Drugs). Incorporates *Farmaco, Edizione Scientifica* [*Farmaco, Ed. Sci.*] (1953–88; FRPSAX)

Finnish Chemical Letters [*Finn. Chem. Lett.*] (1974–89; FCMLAS). No longer published

Gazzetta Chimica Italiana [*Gazz. Chim. Ital.*] (1871–; GCITA9)

Helvetica Chimica Acta [*Helv. Chim. Acta*] (1918–; HCACAV)

Heteroatom Chemistry [*Heteroatom Chem.*] (1990–; HETCE8)

Heterocycles [*Heterocycles*] (1973–; HTCYAM)

Hoppe-Seylers Zeitschrift für Physiologische Chemie see *Biological Chemistry Hoppe-Seyler*

Huaxue Xuebao [*Huaxue Xuebao*] (1953–; HHHPA4) (Journal of Chemistry). In Chinese. Formerly *Journal of the Chinese Chemical Society* [*J. Chin. Chem. Soc. (Peking)*] (1933–52). There is an English edition called *Chinese Journal of Chemistry* [*Chin. J. Chem.*] (1990–; CJOCEV), formerly *Acta Chimica Sinica* [*Acta Chim. Sin. (Engl. Ed.)*] (1983–89; ACSIEW)

Hungarica Acta Chimica see *Acta Chimica Hungarica*

Indian Journal of Chemistry [*Indian J. Chem.*] (1963–75; IJOCAP). In 1976, divided into Section A [*Indian J. Chem., Sect. A*] (1976–; IJCADU, ICACEC) (inorganic, bio-inorganic, physical, theoretical and analytical) and Section B [*Indian J. Chem., Sect. B*] (1976–; IJSBDB) (organic and medicinal). *Indian Journal of Chemistry* was a successor to *Journal of Scientific and Industrial Research* [*J. Sci. Ind. Res.*] (1942–62), which from 1946–62 was divided into: Section A [*J. Sci. Ind. Res., Sect. A*] (general); Section B [*J. Sci. Ind. Res., Sect. B*] (physical sciences); and Section C [*J. Sci. Ind. Res., Sect. C*] (biological sciences)

Indian Journal of Heterocyclic Chemistry [*Indian J. Heterocycl. Chem.*] (1991–; IJCHEI)

Inorganica Chimica Acta [*Inorg. Chim. Acta*] (1967–; ICHAA3)

Inorganic and Nuclear Chemical Letters see *Polyhedron*

Inorganic Chemistry [*Inorg. Chem.*] (1962–; INOCAJ)

International Journal of Peptide and Protein Research [*Int. J. Pept. Protein Res.*] (1972–; IJPPC3). Formerly *International Journal of Protein Research* [*Int. J. Protein Res.*] (1969–72; IPRRBQ)

International Journal of Sulfur Chemistry see *Phosphorus, Sulfur and Silicon and the Related Elements*

Israel Journal of Chemistry [*Isr. J. Chem.*] (1963–; ISJCAT). Successor to *Bulletin of the Research Council of Israel* [*Bull. Res. Counc. Isr.*] (1951–55) and its subsequent Section A [*Bull. Res. Counc. Isr., Sect. A*] (1955–63) (1955–57, maths, physics and chemistry; 1957–63, chemistry)

Izvestiya Akademii Nauk, Seriya Khimicheskaya [*Izv. Akad. Nauk, Ser. Khim.*] (1936–; IASKA6). In Russian. Until 1992, the title was *Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya* [*Izv. Akad. Nauk SSSR, Ser. Khim.*] (IASKA6). There is an English translation called *Russian Chemical Bulletin* [*Russ. Chem. Bull.*] (1993–), formerly *Bulletin of the Academy of Sciences of the USSR, Division of Chemical Sciences* [*Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*] (BACCAT)

Japanese Journal of Antibiotics see *Journal of Antibiotics*

Japanese Journal of Chemistry see *Nippon Kagaku Kaishi*

Journal de Pharmacie et de Chimie see *Annales Pharmaceutiques Français*

Journal für Praktische Chemie – Chemiker-Zeitung [*J. Prakt. Chem./Chem. Ztg.*] (vol. 334; 1992–; JPCCEM). Formed by a merger of *Journal für Praktische Chemie* [*J. Prakt. Chem.*] (1834–1991; JPCEAO) and *Chemiker-Zeitung* [*Chem.-Ztg.*] (1879–1991; CMKZAT)

Journal of Agricultural and Food Chemistry [*J. Agric. Food Chem.*] (1953–; JAFCAU)

Journal of Antibiotics [*J. Antibiot.*] (1948–; JANTAJ). English translation of the Japanese-language journal *Japanese Journal of Antibiotics* [*Jpn. J. Antibiot.*] (JJANAX). From 1953–67 published as Series A [*J. Antibiot., Ser. A*] (English language) and Series B [*J. Antibiot., Ser. B*] (Japanese language)

Journal of Biochemistry [*J. Biochem. (Tokyo)*] (1922–; JOBIAO)

Journal of Biological Chemistry [*J. Biol. Chem.*] (1905–; JBCHA3)

Journal of Carbohydrate Chemistry [*J. Carbohydr. Chem.*] (1982–; JCACDM). Successor to *Journal of Carbohydrates, Nucleosides, and Nucleotides* [*J. Carbohydr., Nucleosides, Nucleotides*] (1974–81; JCNNAF), which was divided into *Journal of Carbohydrate Chemistry* and *Nucleosides and Nucleotides* [*Nucleosides Nucleotides*] (1982–; NUNUD5)

Journal of Chemical Education [*J. Chem. Educ.*] (1924–; JCEDA8)

Journal of Chemical Research (1977–). Consists of two parts: Part M, a miniprint/microfiche, full-text version [*J. Chem. Res. (M)*] (JRMPDM); and Part S, a synopsis version [*J. Chem. Res. (S)*] (JRPSDC). No volume numbers

Journal of Chemistry of the United Arab Republic see *Egyptian Journal of Chemistry*

Journal of Fluorine Chemistry [*J. Fluorine Chem.*] (1971–; JFLCAR)

Journal of General Chemistry of the USSR see *Zhurnal Obshchei Khimii*

Journal of Heterocyclic Chemistry [*J. Heterocycl. Chem.; J. Het. Chem.* in DOC 6] (1964–; JHTCAD)

Journal of Labelled Compounds and Radiopharmaceuticals [*J. Labelled Compd. Radiopharm.*] (1976–; JLCRD4). Formerly *Journal of Labelled Compounds* [*J. Labelled Compd.*] (1965–75; JLCAAI)

Journal of Lipid Research [*J. Lipid Res.*] (1959–; JLPRAW)

Journal of Magnetic Resonance [*J. Magn. Reson.*] (1969–92; JOMRA4). Now divided into Series A [*J. Magn. Reson., Ser. A*] (1993–; JMRAE2); and Series B [*J. Magn. Reson., Ser. B*] (1993–; JMRBE5)

Journal of Mass Spectrometry [*J. Mass Spectrom.*] (1995–). Formerly *Organic Mass Spectrometry* [*Org. Mass Spectrom.*] (1968–94; ORMSBG). Incorporates *Biological Mass Spectrometry* [*Biol. Mass Spectrom.*] [1991–94; BIMSEH]: formerly *Biomedical Mass Spectrometry* [*Biomed. Mass Spectrom.*] (1974–85; BMSYAL); and *Biomedical and Environmental Mass Spectrometry* [*Biomed. Environ. Mass Spectrom.*] (1986–; BEMSEN)

Journal of Medicinal Chemistry [*J. Med. Chem.*] (1963–; JMCMAR). Formerly *Journal of Medicinal and Pharmaceutical Chemistry* [*J. Med. Pharm. Chem.*] (1959–62)

Journal of Medicinal Plant Research see *Planta Medica*

Journal of Molecular Structure [*J. Mol. Struct.*] (1967–; JMOSB4). From 1981 onwards, some volumes have been published as *THEOCHEM* [*THEOCHEM*] (THEODJ); each of these volumes has a *Journal of Molecular Structure* volume number and a different *THEOCHEM* volume number

Journal of Natural Products [*J. Nat. Prod.*] (1979–; JNPRDF). Formerly *Lloydia* [*Lloydia*] (1938–78; LLOYA2)

Journal of Organic Chemistry [*J. Org. Chem.*; *J.O.C.* in DOC 6] (1936–; JOCEAH)

Journal of Organic Chemistry of the USSR see *Zhurnal Organicheskoi Khimii*

Journal of Organometallic Chemistry [*J. Organomet. Chem.*] (1963–; JORCAI)

Journal of Pharmaceutical Sciences [*J. Pharm. Sci.*] (1961–; JPMSAE)

Journal of Pharmacy and Pharmacology [*J. Pharm. Pharmacol.*] (1929–; JPPMAB). From 1929–48, the title was *Quarterly Journal of Pharmacy and Pharmacology* [*Q. J. Pharm. Pharmacol.*]

Journal of Physical Organic Chemistry [*J. Phys. Org. Chem.*] (1988–; JPOCEE)

Journal of Scientific and Industrial Research see *Indian Journal of Chemistry*

Journal of Steroid Biochemistry and Molecular Biology [*J. Steroid Biochem. Mol. Biol.*] (1990–; JSBBEZ). Formerly *Journal of Steroid Biochemistry* [*J. Steroid Biochem.*] (1969–90; JSTBBK)

Journal of Synthetic Organic Chemistry see *Yuki Gosei Kagaku Kyokaishi*

Journal of the American Chemical Society [*J. Am. Chem. Soc.*; J.A.C.S. in DOC 6] (1879–; JACSAT). Absorbed *American Chemical Journal* [*Am. Chem. J.*] (1879–1913)

Journal of the Chemical Society [*J. Chem. Soc.*; *J.C.S.* in DOC 6] (1849–1965). From 1849–61, the title was *Quarterly Journal, Chemical Society* [*Q. J., Chem. Soc.*] (1849–1861). Volume numbers were used until 1927 (vol. 128). In 1966, divided into Part A [*J. Chem. Soc. A*; *J.C.S. A* in DOC 6] (1966–71) (inorganic); Part B [*J. Chem. Soc. B*; *J.C.S. B* in DOC 6] (1966–71) (physical organic); and Part C [*J. Chem. Soc. C*; *J.C.S. C* in DOC 6] (1966–71) (organic). *Chemical Communications* [*Chem. Comm.*] (1965–69, CCOMA8) became Part D [*J. Chem. Soc. D*] (1970–71). In 1972, Parts A–D were superseded by *Dalton Transactions* [*J. Chem. Soc., Dalton Trans.*; *J.C.S. Dalton* in DOC 6] (1972–; JCDTBI) (inorganic); *Perkin Transactions 1* [*J. Chem. Soc., Perkin Trans. 1*; *J.C.S. Perkin 1* in DOC 6] (1972–; JCPRB4) (organic and bio-organic); *Perkin Transactions 2* [*J. Chem. Soc., Perkin Trans. 2*; *J.C.S. Perkin 2* in DOC 6] (1972–; JCPKBH) (physical organic); and *Chemical Communications* [*J. Chem. Soc., Chem. Commun.*; *Chem. Comm.* in DOC 6] (1972–; JCCCAT) (preliminary communications), respectively. At the same time, *Transactions of the Faraday Society* [*Trans. Faraday Soc.*] was divided into two parts, which became sections of *Journal of the Chemical Society*: *Faraday*

Transactions 1 [*J. Chem. Soc., Faraday Trans. 1*; *J.C.S. Faraday 1* in DOC 6] (1972–89; JCFTAR); and *Faraday Transactions 2* [*J. Chem. Soc., Faraday Trans. 2*; *J.C.S. Faraday 2* in DOC 6] (1972–89; JCFTBS); in 1990 they were merged to form *Faraday Transactions* [*J. Chem. Soc., Faraday Trans.*] (1990–; JCFTEV). Only *Faraday Transactions* has volume numbers

Journal of the Chemical Society of Japan see *Nippon Kagaku Kaishi*

Journal of the Chemical Society of Pakistan [*J. Chem. Soc. Pak.*] (1979–; JCSPDF)

Journal of the Chinese Chemical Society (Peking) see *Huaxue Xuebao*

Journal of the Chinese Chemical Society (Taipei) [*J. Chin. Chem. Soc. (Taipei)*] (1954–; JCCTAC). In English

Journal of the Indian Chemical Society [*J. Indian Chem. Soc.*] (1924–; JICSAH). From 1924–27, the title was *Quarterly Journal of the Indian Chemical Society* [*Q. J. Indian Chem. Soc.*]

Journal of the Pharmaceutical Society of Japan see *Yakugaku Zasshi*

Journal of the Royal Netherlands Chemical Society see *Recueil des Travaux Chimiques des Pays-Bas*

Journal of the Science of Food and Agriculture [*J. Sci. Food Agric.*] (1950–; JSFAAE)

Journal of the Society of Chemical Industry see *Chemistry and Industry*

Journal of the South African Chemical Institute see *South African Journal of Chemistry*

Justus Liebigs Annalen der Chemie see *Liebigs Annalen*

Khimiya Geterotsiklicheskikh Soedinenii [*Khim. Geterotsikl. Soedin.*] (1965–; KGSSAQ). In Russian. There is an English translation called *Chemistry of Heterocyclic Compounds* [*Chem. Heterocycl. Compd. (Engl. Transl.)*] (1965–; CHCCAL)

Khimiya Prirodnykh Soedinenii [*Khim. Prir. Soedin.*] (1965–; KPSUAR). In Russian. There is an English-language translation called *Chemistry of Natural Compounds* [*Chem. Nat. Compd. (Engl. Transl.)*] (1965–; CHNCA8)

Liebigs Annalen [*Liebigs Ann.*; *Annalen* in DOC 6] (1840–). Former titles are: *Annalen der Chemie und Pharmazie* [*Ann. Chem. Pharm.*] (1840–73); *Justus Liebigs Annalen der Chemie und Pharmazie* [*Justus Liebigs Ann. Chem. Pharm.*] (1873–74); *Justus Liebigs Annalen der Chemie* [*Justus Liebigs Ann. Chem.*] (1875–1978; JLACBF); and *Liebigs Annalen der Chemie* [*Liebigs Ann. Chem.*] (1979–94; LACHDL). Often referred to as *Annalen* [*Ann.*]. Volume numbers used until 1972 (vol. 766). From 1995 accepts papers in English covering organic chemistry only.

Lipids [*Lipids*] (1966–; LPDSAP)

Lloydia see *Journal of Natural Products*

Magnetic Resonance in Chemistry [*Magn. Reson. Chem.*] (vol. 23; 1985–; MRCHEG). Formerly *Organic Magnetic Resonance* [*Org. Magn. Reson.*] (1969–84; ORMRBD)

Magyar Kemiai Folyoirat [*Magy. Kem. Foly.*] (1895–; MGKFA3) (Hungarian Journal of Chemistry). Until 1949, the title was *Magyar Chemiai Folyoirat* [*Magy. Chem. Foly.*]

Mendeleev Communications [*Mendeleev Commun.*] (1991–; MENCEX)

Methods in Carbohydrate Chemistry [*Methods Carbohydr. Chem.*] (1962–; MCACAI). Irregular

Monatshefte für Chemie [*Monatsh. Chem.*] (1880–; MOCMB7). From 1880–1967, the title was *Monatshefte für Chemie und Verwandte Teile Anderer Wissenschaaften* [*Monatsh. Chem. Verw. Teile Anderer Wiss.*]

Natural Product Letters [*Nat. Prod. Lett.*] (1992–; NPLEEF)

Natural Product Reports [*Nat. Prod. Rep.*] (1984–; NPRRDF). Review journal

Nature [*Nature (London)*] (1869–; NATUAS)

Naturwissenschaften [*Naturwissenschaften*] (1913–; NATWAY)

New Journal of Chemistry [*New J. Chem.*] (1987–; NJCHE5). Formerly *Nouveau Journal de Chimie* [*Nouv. J. Chem.*] (1977–86; NJCHD4)

Nippon Kagaku Kaishi [*Nippon Kagaku Kaishi*] (1921–47, 1972–; NKAKB8) (Journal of the Chemical Society of Japan). In Japanese. No English translation is available. From 1948–71, it was replaced by *Nippon Kagaku Zasshi* [*Nippon Kagaku Zasshi*] (Japanese Journal of Chemistry)

Norvegica Pharmaceutica Acta see *European Journal of Pharmaceutical Sciences*

Nouveau Journal de Chimie see *New Journal of Chemistry*

Nucleosides and Nucleotides see *Journal of Carbohydrate Chemistry*

Organic Magnetic Resonance see *Magnetic Resonance in Chemistry*

Organic Mass Spectrometry see *Journal of Mass Spectrometry*

Organic Preparations and Procedures International [*Org. Prep. Proced. Int.*] (1971–; OPPIAK). Formerly *Organic Preparations and Procedures* [*Org. Prep. Proced.*] (1969–70; OGPPAC)

Organometallics [*Organometallics*] (1982–; ORGND7)

Peptides [*Peptides (Fayetteville, N.Y.)*] (1980–; PEPTDO, PPTDD5)

Pharmaceutical Bulletin see *Chemical and Pharmaceutical Bulletin*

Pharmazie [*Pharmazie*] (1946–; PHARAT)

Phosphorus, Sulfur and Silicon and the Related Elements [*Phosphorus, Sulfur Silicon Relat. Elem.*] (1989–; PSSLEC). Formerly *Phosphorus and Sulfur and the Related Elements* [*Phosphorus Sulfur Relat. Elem.*] (1976–88; PREEDF), which was formed by a merger of *Phosphorus and the Related Group V Elements* [*Phosphorus Relat. Group V Elem.*] (1971–76; PHOSAB) and *International Journal of Sulfur Chemistry* [*Int. J. Sulfur Chem.*] (1973–76; IJSCCD). *International Journal of Sulfur Chemistry* was previously divided into: Part A [*Int. J. Sulfur Chem., Part A*] (1971–72; IJTSAU) (original experimental and theoretical studies); Part B [*Int. J. Sulfur Chem., Part B*] (1971–72; IQSCAQ), previously *Quarterly Reports on Sulfur Chemistry* [*Q. Rep. Sulfur Chem.*] (1966–70; QRSCBK); and Part C [*Int. J. Sulfur Chem., Part C*] (1971–72; ISCCBT), previously *Mechanisms of Reactions of Sulfur Compounds* [*Mech. React. Sulfur Compd.*] (1966–70; MRSCA9)

Phytochemistry [*Phytochemistry*] (1961–; PYTCAS)

Planta Medica [*Planta Med.*] (1953–; PLMEAA). Sometimes referred to as *Journal of Medicinal Plant Research: Planta Medica* [*J. Med. Plant Res.: Planta Med.*]

Polish Journal of Chemistry [*Pol. J. Chem.*] (1978–; PJCHDQ). Formerly *Roczniki Chemii* [*Rocz. Chem.*] (1921–77)

Polyhedron [*Polyhedron*] (1982–; PLYHDÉ). Successor to *Journal of Inorganic and Nuclear Chemistry* [*J. Inorg. Nucl. Chem.*] (1955–81; JINCAO) and *Inorganic and Nuclear Chemistry Letters* [*Inorg. Nucl. Chem. Lett.*] (1965–81; INUCAF)

Proceedings of the Chemical Society, London [*Proc. Chem. Soc., London*] (1885–1914, 1957–64; PCSLAW). From 1915–56 there was a Proceedings section in *Journal of the Chemical Society*

Proceedings of the National Academy of Sciences of the United States of America [*Proc. Natl. Acad. Sci. U.S.A.*] (1863–; PNASA6)

Prostaglandins [*Prostaglandins*] (1972–; PRGLBA)

Pure and Applied Chemistry [*Pure Appl. Chem.*] (1960–; PACHAS)

Quarterly Reviews of the Chemical Society see *Chemical Society Reviews*

Recueil des Travaux Chimiques des Pays-Bas [*Recl. Trav. Chim. Pays-Bas*; *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)* in DOC 6] (1882; RTCPA3). Also known as *Journal of the Royal Netherlands Chemical Society* [*J. R. Neth. Chem. Soc.*]. From 1897–1919, the title was *Recueil des Travaux Chimiques des Pays-Bas et de la Belgique* [*Recl. Trav. Chim. Pays-Bas Belg.*]

Revue Roumaine de Chimie [*Rev. Roum. Chem.*] (1964–; RRCHAX). Formerly *Revue de Chimie, Académie de la République Populaire Roumaine* [*Rev. Chim. Acad. Repub. Pop. Roum.*] (1954–63)

Roczniki Chemii see *Polish Journal of Chemistry*

Russian Chemical Bulletin see *Izvestiya Akademii Nauk, Seriya Khimicheskaya*

Russian Chemical Reviews see *Uspekhi Khimii*

Russian Journal of Applied Chemistry see *Zhurnal Prikladnoi Khimii*

Russian Journal of General Chemistry see *Zhurnal Obshchei Khimii*

Russian Journal of Inorganic Chemistry see *Zhurnal Neorganicheskoi Khimii*

Russian Journal of Organic Chemistry see *Zhurnal Organicheskoi Khimii*

Science [*Science (Washington, D.C.)*] (1883–; SCIEAS)

Scientia Pharmaceutica [*Sci. Pharm.*] (1930–; SCPHA4)

South African Journal of Chemistry [*S. Afr. J. Chem.*] (1977–; SAJCDC). Formerly *Journal of the South African Chemical Institute* [*J. S. Afr. Chem. Inst.*] (1922–76; JSACAT)

Soviet Journal of Bioorganic Chemistry see *Bioorganicheskaia Khimia*

Spectrochimica Acta [*Spectrochim. Acta*] (1939–66;

SPACA5). From vol. 23, divided into: Part A [*Spectrochim. Acta, Part A*; *Spectrochim. Acta A* in DOC 6] (1967–; SAMCAS) (molecular spectroscopy); and Part B [*Spectrochim. Acta, Part B*; *Spectrochim. Acta B* in DOC 6] (1967–; SAASBH) (atomic spectroscopy)

Steroids [*Steroids*] (1963–; STEDAM)

Synlett [*Synlett*] (1989–; SYNLES)

Synthesis [*Synthesis*] (1969–; SYNTBF). No volume numbers

Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry [*Synth. React. Inorg. Met.-Org. Chem.*] (1974–; SRIMCN). Formerly *Synthesis in Inorganic and Metal-Organic Chemistry* [*Synth. Inorg. Met.-Org. Chem.*] (1971–73; SIMOAI)

Synthetic Communications [*Synth. Commun.*] (1971–; SYNCAV)

Tetrahedron [*Tetrahedron*] (1957–; TETRAB)

Tetrahedron: Asymmetry [*Tetrahedron: Asymmetry*] (1990–; TASYE3)

Tetrahedron Letters [*Tetrahedron Lett,; Tet. Lett.* in DOC 6] (1959–; TELEAY). Volume numbers first used with vol. 21 (1980)

THEOCHEM see *Journal of Molecular Structure*

United Arab Republic Journal of Chemistry see *Egyptian Journal of Chemistry*

Uspekhi Khimii [*Usp. Khim.*] (1932–; USKHAB). In Russian. There is an English translation entitled *Russian Chemical Reviews* [*Russ. Chem. Rev. (Engl. Transl.)*] (1960–; RCRVAB)

Yakugaku Zasshi [*Yakugaku Zasshi*] (1881–; YGKKAE). Also known as *Journal of the Pharmaceutical Society of Japan*. In Japanese. No English translation is available

Yuki Gosei Kagaku Kuokaishi (1943–; YGKKAE). Also known as *Journal of Synthetic Organic Chemistry* [*J. Synth. Org. Chem.*]. In Japanese. No English translation is available

Zeitschrift für Angewandte Chemie see *Angewandte Chemie*

Zeitschrift für Anorganische und Allgemeine Chemie [*Z. Anorg. Allg. Chem.*] (1892–; ZAACAB). From 1892–95 and 1943–50, the title was *Zeitschrift für Anorganische Chemie* [*Z. Anorg. Chem.*]

Zeitschrift für Chemie see *Angewandte Chemie*

Zeitschrift für Kristallographie [*Z. Kristallogr.*] (1877–; ZEKRDZ). Formerly titled *Zeitschrift für Kristallographie und Mineralogie* [*Z. Kristallogr. Mineral.*] (1877–1915) and *Zeitschrift für Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie* [*Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*] (1921–77; ZKKKAJ)

Zeitschrift für Naturforschung [*Z. Naturforsch.*] (1946). In 1947, divided into Teil A [*Z. Naturforsch., A*] (1947–; ZENAAU, ZTAKDZ, ZNASEI) (physical sciences); and Teil B [*Z. Naturforsch., B*] (1947–; ZENBAX, ZNBAD2, ZNBSEN) (chemical sciences); to which was later added Teil C [*Z. Naturforsch., C*] (1973–; ZNFCAP, ZNCBDA) (biosciences – previously included in Teil B)

Zhurnal Neorganicheskoi Khimii [*Zh Neorg. Khim.*] (1956–; ZNOKAQ). In Russian. There is an English translation called *Russian Journal of Inorganic Chemistry* [*Russ. J. Inorg. Chem.*] (1959–; RJICAQ). Formerly *Journal of Inorganic Chemistry (USSR)* [*J. Inorg. Chem. (USSR)*] (1956–58)

Zhurnal Obshchei Khimii [*Zh. Obshch. Khim.*] (1931–; ZOKHA4). In Russian. There is an English translation called *Russian Journal of General Chemistry* [*Russ. J. Gen. Chem.*] (1993–). Formerly *Journal of General Chemistry of the USSR* [*J. Gen. Chem. USSR (Engl. Transl.)*] (1949–92; JGCHA4)

Zhurnal Organicheskoi Khimii [*Zh. Org. Khim.*] (1965–; ZORKAE). In Russian. There is an English translation called *Russian Journal of Organic Chemistry* [*Russ. J. Org. Chem.*] (1993–). Formerly *Journal of Organic Chemistry of the USSR* [*J. Org. Chem. USSR (Engl. Transl.)*] (1965–92; JORCAI)

Zhurnal Prikladnoi Khimii [*Zh. Prikl. Khim. (Leningrad)*] (1928–; ZPKHAB). In Russian. There is an English translation called *Russian Journal of Applied Chemistry* [*Russ. J. Appl. Chem.*] (1993–). Formerly *Journal of Applied Chemistry of the USSR* [*J. Appl. Chem. USSR (Engl. Transl.)*] (1950–92; JAPUAW)

4 Useful reference works in organic chemistry

This list comprises some of the more important reference books and series of books dealing with organic compounds. For major abstracting and indexing publications, such as *Chemical Abstracts* and *Beilstein*, see the next chapter.

Advanced Organic Chemistry; Reactions, Mechanisms and Structures, 4th edn, J. March (Wiley, 1992).

The Agrochemicals Handbook (Royal Society of Chemistry). See below under *Pesticide Manual*.

Atlas of Stereochemistry, 2nd edn, W. Klyne and J. Buckingham, 2 vols (Chapman & Hall, 1978); suppl. by J. Buckingham and R.A. Hill (Chapman & Hall, 1986). The standard reference for absolute configuration determinations up to 1982.

Carbohydrates, ed. P.M. Collins (Chapman & Hall, 1987). A desktop reference including all carbohydrate entries from the Chapman & Hall database at the time of publication.

Chemistry of Functional Groups, ed. S. Patel (Wiley, 1964–). A series of volumes. Each volume covers all aspects of the chemistry of individual functional groups important in organic chemistry.

Chemical Abstracts Ring Systems Handbook (American Chemical Society, 1993). Provides names and formulae of rings published in *Chemical Abstracts*. Supersedes earlier publications, such as *The Ring Index*; cumulative supplements are issued bi-annually.

The Chemistry of Heterocyclic Compounds; A Series of Monographs, ed. A. Weissberger, 1950–70; eds A. Weissberger and E.C. Taylor, 1970– (Interscience). Comprehensive coverage of the complete field of heterocyclic chemistry. Each volume deals with one or more ring systems.

Compendium of Chemical Terminology; IUPAC Recommendations, eds V. Gold *et al.* (Blackwell Scientific, 1987).

Comprehensive Heterocyclic Chemistry: The Structure, Reactions, Synthesis and Uses of Heterocyclic Compounds, eds A.R. Katritzky and C.W. Rees, 8 vols (Pergamon, 1984).

Comprehensive Medicinal Chemistry: The Rational Design, Mechanistic Study and Therapeutic Applications of Chemical Compounds, ed. C. Hansch, 6 vols (Pergamon, 1990).

Comprehensive Organic Chemistry: The Synthesis and Reactions of Organic Compounds, eds D.H.R. Barton and W.D. Ollis, 6 vols (Pergamon, 1979).

Comprehensive Organic Synthesis: Selectivity, Strategy and Efficiency in Modern Organic Chemistry, eds B.M. Trost and I. Fleming, 9 vols (Pergamon, 1991).

Comprehensive Organometallic Chemistry: The Synthesis, Reactions and Structures of Organometallic Compounds, eds G. Wilkinson, F.G.A. Stone and E.W. Abel, 9 vols (Pergamon, 1982). Second Edition to appear in 1995 or 1996.

Dictionary of Alkaloids, eds I.W. Southon and J. Buckingham, 2 vols (Chapman & Hall, 1989). Presents structure, physical properties, biological source and bibliographic data on around 10 000 alkaloids within 5000 entries. Now superseded by *Dictionary of Natural Products*.

Dictionary of Antibiotics and Related Substances, ed. B.W. Bycroft (Chapman & Hall, 1987). Contains structure, property and bibliographic data on around 8000 significant antibiotics.

Dictionary of Drugs, eds J. Elks and C.R. Ganellin, 2 vols (Chapman & Hall, 1990). Includes information on more than 6000 drugs.

Dictionary of Natural Products, ed. J. Buckingham, 7 vols (Chapman & Hall, 1994). Contains chemical, structural and bibliographic data for 100 000 natural products and related compounds, grouped into 34 000 entries of closely related substances. Annual supplements are to be issued. Volume 7 contains a long introductory section giving accepted representations and numbering of all natural product carbon skeletons.

Dictionary of Organometallic Compounds, ed. J. Macintyre, 2nd edn, 5 vols (Chapman & Hall, 1995). Contains data on over 40 000 organometallics.

Dictionary of Organophosphorus Compounds, ed. R.S. Edmundson (Chapman & Hall, 1988). Gives structure, property and bibliographic data on 20 000 organophosphorus compounds.

Dictionary of Steroids, eds D.N. Kirk, R.A. Hill, H.L.J. Makin and G.M. Murphy, 2 vols (Chapman & Hall, 1991). Presents physical and chemical data, biological source and medicinal uses for over 15 000 steroids in 6000 entries.

Dictionary of Terpenoids, eds J.D. Connolly and R.A. Hill (Chapman & Hall, 1991). Contains information on over 20 000 terpenoids. Now superseded by *Dictionary of Natural Products*.

Elsevier's Encyclopaedia of Organic Chemistry, ed. F. Radt (Elsevier, 1940–56; Springer, 1959–69). Only volumes 12–14 (*Condensed Carbisocyclic Compounds*) were published. Publication was suspended in 1956, but further supplements were published by Springer until the steroid sections in *Beilstein* appeared. A good entry to the old literature on naphthalenes, anthracenes, etc.

Encyclopedia of Reagents for Organic Synthesis, 8 vols (Wiley, 1995). Reviews almost 3500 reagents.

Fortschritte der Chemie Organischer Naturstoffe (Progress in the Chemistry of Organic Natural Products) (Springer, 1938–). A series of volumes containing reviews on classes of natural products.

A Guide to IUPAC Nomenclature of Organic Compounds, R. Panico *et al.* (Blackwell Scientific, 1993).

Kirk-Othmer Encyclopedia of Chemical Technology, 3rd edn, 24 vols + suppl. vol. + index vol. (1978–84). The 4th edition (1991–) is currently being published. Despite its title, this encyclopaedia contains much pure chemistry.

Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn, W. Karrer (Birkhäuser, 1976). Gives a complete record of all natural products (except alkaloids) up to about 1966.

The Lipid Handbook, 2nd edn, eds F.D. Gunstone, J.L. Harwood and F.B. Padley (Chapman & Hall, 1994). Gives physical properties and literature references for over 3000 lipids and their derivatives.

Martindale, The Extra Pharmacopoeia, 30th edn (Pharmaceutical Press, 1993). Contains monographs on drugs and ancillary substances.

The Merck Index; An Encyclopedia of Chemicals, Drugs and Biologicals, 11th edn (Merck, 1989). A handy, one-volume compendium of information on the most important chemicals, drugs and biological substances (10 100 entries).

Methoden der Organischen Chemie, Houben-Wehl (Georg Thieme, 1952). In German. Complete in 16 volumes (volume 16 is an index volume).

Methods in Enzymology (Academic Press, 1955–). This ongoing series of books now numbers over 230 volumes, each devoted to a specific aspect of enzymology.

Organic Reactions (Wiley, 1942–). This series contains review chapters, each devoted to a single reaction of wide applicability.

Organic Synthesis (Wiley, 1921–). Annual series giving checked and edited experimental procedures that illustrate new synthetic methods or describe the preparation of particularly useful compounds. Collective volumes are issued containing revised editions of sets of annual volumes.

The Pesticide Manual: Incorporating the Agrochemicals Handbook, 10th edn (British Crop Protection Council, 1994).

Protective Groups in Organic Synthesis, 2nd edn, T.W. Greene and P.G.M. Wuts (Wiley-Interscience, 1991).

Reagents for Organic Synthesis, L.F. Fieser and M. Fieser (1967–86); M. Fieser and J.G. Smith (1988–). Reagents used in organic synthesis are listed alphabetically.

Rodd's Chemistry of Carbon Compounds, 2nd edn, ed. S. Coffey (Elsevier, 1964–89); suppl. to 2nd edn, ed. M.F. Ansell (1973–); 2nd suppl. to 2nd edn, ed. M. Sainsbury (1991–). Contains general information on organic chemistry.

Complete in 5 volumes, each volume being in several parts. Volume 5 is a general index. An excellent source of review data on various classes of compounds, although the indexes are now cumbersome.

Theilheimer's Synthetic Methods of Organic Chemistry, A.F. Finch (1982–); formerly *Synthetic Methods of Organic Chemistry*, W. Theilheimer (Karger, 1948–81). Abstracts new methods for the synthesis of organic compounds. Reactions are classified on a simple though purely formal basis by symbols, which can be arranged systematically. A subject index lists reaction names (e.g. Fries rearrangement) and types of compounds (starting materials and end-products).

Ullmann's Encyclopedia of Industrial Chemistry, 5th edn (VCH, 1985–). Previous editions from the 1st edition (1914) to the 4th edition (1972–84) were published in German. The 5th edition is in English and commenced publication in 1985. It consists of two parts. Part A, which is in alphabetical order, consists of 28 volumes. Part B consists of 8 volumes covering fundamental techniques in industrial chemistry.

5 Abstracting and indexing publications

5.1 *Chemical Abstracts*

Chemical Abstracts (CA) has referenced over 14 million documents since 1907. It is the most comprehensive single source of information about chemistry and chemical compounds.

Each week, CA carries over 10 000 abstracts. CA covers items from scientific and technical journals, patent documents, conference and symposium proceedings, dissertations, government reports and books. Abstracts in CA are placed in one of 80 sections based upon their subject matter. The sections are collected into five broad groupings: Biochemistry (sections 1–20), Organic chemistry (21–34), Macromolecular chemistry (35–46), Chemistry and chemical engineering (47–64) and Physical, inorganic and analytical chemistry (65–80). Sections 1–34 are published one week (odd-numbered issues) and sections 35–80 the following week (even-numbered issues). At the end of each issue appear indexes of: (1) author names; (2) keyword phrases chosen from the abstract text and document titles; and (3) patent numbers.

CA Volume Indexes, published every six months, are in-depth indexes whose entries are selected from the original documents, not just the abstracts. Every five years the Volume Indexes are merged and republished as a single index to all abstracts published during that five years; this is known as a Collective Index (CI). Before 1957, Collective Indexes covered 10 years and were called Decennial Indexes (DI). Table 5.1 gives details of Decennial and Collective Indexes.

The *Index Guide* provides cross-references to various chemical substance names and general subject terms to the controlled terminology employed in the current Volume Indexes and also gives details of the major points of indexing policy. It was first published with the 8CI in 1968. Before then, cross-references were included in the Subject Indexes themselves.

The *General Subject Index* contains subject terms referring to reactions, processes and equipment; classes of substances; and plant and animal species. Before using the General Subject Index, the Index Guide should be consulted in order to determine the correct index headings. Before 1972, general subjects and chemical substances appeared together in a Subject Index.

Table 5.1 CA Decennial and Collective Indexes

Index	Years	Volumes
1st DI	1907–16	1–10
2nd DI	1917–26	11–20
3rd DI	1927–36	21–30
4th DI	1937–46	31–40
5th DI	1947–56	41–50
6th CI	1957–61	51–55
7th CI	1962–66	56–65
8th CI	1967–71	66–75
9th CI	1972–76	76–85
10th CI	1977–81	86–95
11th CI	1982–86	96–105
12th CI	1987–91	106–115
13th CI	1992–96	116–125

The *Chemical Substance Index* is an index of chemical substances arranged alphabetically by CA Index Name (see Section 7.2). One thing to remember when doing a retrospective search is that the Index Name of a substance may change between collective periods. For example, the same substance may appear under different names in 7CI, 8CI and 9CI; for a list equating 9CI names with the corresponding 8CI names, see Section 7.3. From 9CI onwards, the Index Name for an organic compound will almost certainly have remained the same. Before 1972, general subjects and chemical substances appeared together in a Subject Index.

The *Formula Index* lists molecular formulae arranged in Hill system order (see Chapter 9). Very early volumes of CA do not have a Formula Index. There is a Collective Formula Index that covers vols 14–40 (1920–46); from then on, each Decennial/Collective Index includes a Formula Index. For some conventions used in the CA Formula Indexes, see Chapter 9.

The *Index of Ring Systems* includes entries for each ring system that CAS encounters during a volume or

collective period. CAS also produces the *Ring Systems Handbook*, which is a comprehensive listing of ring systems (see section 8.2 under **ring systems**).

There is also an *Author Index* and a *Patent Index*. See Chapter 6 for some information about patents.

5.2 *Chemisches Zentralblatt*

Founded in 1830, this German language abstracting publication was discontinued in 1969. It is considered superior to *Chemical Abstracts*, giving more detailed abstracts and abstracting from sources not covered by CAS. It can still be useful for searching the old literature, although *Beilstein* is more convenient when searching for information on specific organic compounds.

5.3 *Beilstein*

Beilstein is the short name of *Beilstein's Handbuch der Organischen Chemie*, which provides a collection of critically examined data on known compounds of carbon. The 4th edition of *Beilstein* has been in print since 1918. It contains information on the preparation and properties of all carbon compounds that were published in the scientific literature over set periods. The complete work is divided into series covering the periods listed in Table 5.2.

The Basic Series and Supplementary Series E I to E IV are in German. Supplementary Series E V, which started publication in 1984, is in English.

Each of the series comprises 27 volumes (or groups of volumes) in which the individual compounds are arranged according to the *Beilstein* system. The *Beilstein* system comprises a set of rules that determine the ordering of the compounds according to their structural features; using the system, any given molecule can be allotted a unique place in the handbook. Volumes 1–4 cover acyclic compounds, 5–16 alicyclic compounds and 17–27 heterocyclic compounds.

The classification of the subject matter in each of the supplementary volumes is the same as that in the 27 volumes of the Basic Series; this means that any particular volume of each Supplementary Series always contains the same classes of compounds (and only these) as the volume of the Basic Series with the same number.

The easiest way to locate a compound in *Beilstein* is to use one of the *Cumulative Indexes*. There have been two of these. The first covers all the compounds described in Series H, E I and E II (literature up to the end of 1929). It comprises a General Subject Index (Sachregister, E II, vol. 28, 2 subvolumes) and a General Formula Index (Formelregister, E II, vol. 29, 3 subvolumes). This index is extremely useful for finding information from old literature, especially that published in the years not covered by *Chemical Abstracts* Formula Indexes (pre-1920).

Formulae in the General Formula Index are arranged according to the Hill system (see Chapter 9), although it should be noted that, in the actual *Beilstein* volumes covered by that index, the Hill system is not followed (e.g. O precedes N). Substances under each formula are listed in the order in which they appear in *Beilstein*, i.e. substances that

Table 5.2 The series of the Beilstein handbook

Series	Abbrev.	Years covered	Colour[a]
Basic Series (Hauptwerk)	H	up to 1910	green
Supplementary Series I	E I	1910–19	dark red
Supplementary Series II	E II	1920–29	white
Supplementary Series III	E III	1930–49	blue
Supplementary Series III/IV	E III/IV[b]	1930–59	blue/black
Supplementary Series IV	E IV	1950–59	black
Supplementary Series V	E V	1960–79	red

[a] The colour refers to the colour of the label on the spine of the books. Series H to E IV are bound in brown. Series E V is bound in blue.

[b] Volumes 17–27 of Supplementary Series III and IV covering the heterocyclic compounds are combined in a joint issue.

are to be found in vol. 1 appear before those to be found in vol. 2, etc. The appropriate volume and page numbers are then given. Thus, in the Formula Index under C_8H_7Br can be found 'ω-Brom-styrol **5** 477, I 230, II 368'. This indicates that information on ω-bromostyrene (PhCH=CHBr) can be found on p. 477 in vol. 5 of the Hauptwerk, on p. 230 in vol. 5 of the First Supplementary Series and on p. 368 in vol. 5 of the Second Supplementary Series.

The second cumulative index is a Centennial Index covering all compounds described in Series H to E IV (literature up to the end of 1959). The General Subject Index (E IV, vol. 28) comprises 10 subvolumes and the General Formula Index (E IV, vol. 29) 13 subvolumes.

Further information, including a user's guide to *Beilstein*, are available from the Beilstein Institute, Carl Bosch Haus, Varrentrappstr. 40-42, D-6000 Frankfurt/M90, Germany.

5.4 Other publications

5.4.1 *Index Chemicus*

Published by the Institute for Scientific Information, *Index Chemicus* is a weekly guide to new organic compounds and their chemistry and is aimed at researchers in organic chemistry and the pharmaceutical industry. It covers just over 100 of the world's leading chemistry and pharmaceutical journals and claims to give comprehensive coverage of over 90% of all significant new organic compounds. It contains abstracts of articles reporting the synthesis and isolation of new compounds. Structural diagrams and reaction schemes are used extensively. Each issue includes five indexes, which are cumulated annually: a Journal Index (a listing of all publications covered), an Author Index, a Biological Activity Index (a guide to those compounds with proven or potential biological applications or activities), an Unisolated Intermediate Index (a listing of all intermediates by class or by reaction type), and a Labeled Compound Index (a listing of all newly synthesised labelled compounds).

5.4.2 *Science Citation Index*

Authors of a scientific document will cite some previous publications, usually giving these as a reference list appended at the end of the document. A citation index is an index of these references. Thus, if a paper by the author A. Smith cites an earlier work by the author B. Jones, then looking up B. Jones's paper in a citation index will lead to A. Smith's paper.

Published by the Institute for Scientific Information (ISI), the *Science Citation Index* covers about 3500 core periodicals covering the whole of science. To use it, you must start with a journal article that is of interest. You can then find all subsequent papers in which that article is cited.

ISI also issue a *Chemistry Citation Index* on CD-ROM.

5.4.3 *Chemical Titles*

Published by Chemical Abstracts Service, *Chemical Titles* is issued weekly and reproduces the tables of contents of about 800 chemistry journals. It gives an index of keywords from the article titles in the form of a keyword-in-context (KWIC) index. There is also an author index.

5.4.4 *Current Contents*

Published by the Institute for Scientific Information, *Current Contents* reproduces the tables of contents of journals and provides an author index and a title word index. It is divided into several parts, of which the following are of interest in the field of chemistry:

- *Current Contents: Physical, Chemical and Earth Sciences*
- *Current Contents: Life Sciences*
- *Current Contents: Agriculture, Biology and Environmental Sciences*

5.4.5 *CA Selects*

Issued every two weeks, a *CA Selects* reproduces the CA abstracts for all papers on a particular topic covered in *Chemical Abstracts*. No indexes are provided. There are over 200 topics. Those of interest to organic chemists include:

- Amino acids, peptides and proteins
- Asymmetric synthesis and induction
- Beta-lactam antibiotics
- Carbohydrates (chemical aspects)

- Natural product synthesis
- New antibiotics
- Novel natural products
- Novel sulfur heterocycles
- Organofluorine chemistry
- Organometallics in organic synthesis
- Organophosphorus chemistry
- Organosulfur chemistry (journals)
- Porphyrins
- Prostaglandins
- Steroids (chemical aspects)

5.4.6 *Methods in Organic Synthesis* and *Natural Products Updates*

These two bulletins are issued monthly by the Royal Society of Chemistry, and each contains about 200 items a month. *Methods in Organic Synthesis* gives reaction schemes for new synthetic methods reported in the current literature. *Natural Products Updates* covers papers dealing with the isolation, structural determination and synthesis of compounds isolated from natural sources.

[MDL Information Systems (U.K.) Limited, Ground Floor, Building 4, Archipelago, Lyon Way, Camberley, Surrey GU16 5ER, England]

5.5.3 *Trilogy (Drugs of the Future, Drug Data Report* and *Drug News and Perspectives)* from Prous Science Publishers.

Windows-based databases providing recent and retrospective drug information on one CD-ROM. *Drugs of the Future* provides information on the synthesis, literature and patent sources for compounds undergoing research and development.

Drug Data Report gives access to product information, manufacturers, current literature and other information. Together with *Drugs of the Future* 65 000 compounds, with accessible connection tables are covered.

Drug News and Perspectives provides text-searchable information on Research and Development news worldwide.

[Prous Science Publishers, Apartado de Correos 540, 08080 Barcelona, Spain]

5.5 Electronic Publications

5.5.1 *Patent Images – Chemical* and *RetroChem* from Micro Patent

RetroChem provides front-page searching of U.S. chemical patents from 1976–1993 on a single disk. *Patent Images – Chemical* contains facsimiles of patent documents with fully searchable bibliographic fields provided with all structures and diagrams. It is issued about every two weeks, containing approximately 1000 new U.S. patents accumulating to approximately 30 disks per year.

5.5.2 *The Available Chemicals Directory* from MDL, Information Systems, Inc.

A structure-searchable database of commercially available chemicals. It contains supplier information from over 200 catalogues, including chemical names/synonyms and CAS registry numbers.

Updated bi-annually. Release 94.1 contains over 140 000 chemical substances.

5.5.4 CAS Databases available on STN International

Chemical Abstracts Service provide a range of on-line databases covering chemistry and chemistry-related sciences.

CA File® corresponds to printed Chemical Abstracts from 1967 to the present, containing 10 000 000 abstracts and comprising 11 000 000 bibliographic references.

Registry is a structure and text-searchable database containing information on approximately 12 000 000 unique substances, with the associated CAS registry numbers.

MARPAT® allows users to search 200 000 Markush structures from 55 000 chemical patent claims cited in the *CA File*® since 1988.

CASREACT® is a structure and text-searchable organic chemical reaction database. Reactions are selected from journals since 1985 and patents from 1991 covering some 1 000 000 single step and 2 000 000 multi step transformations from the organic chemistry sections of Chemical Abstracts.

CA Previews provides access to article titles and bibliographic information prior to a fully indexed

record appearing in the on-line or printed versions of Chemical Abstracts.

CHEMLIST® is a Regulated Chemicals listing. Regulated substances listed on the Environmental Protection Agency Toxic Substances Control Act Inventory, the European Inventory of Existing Commercial Chemical Substances, and the Domestic and Non-Domestic Substances List from Canada are covered as well as other lists of hazardous substances.

CIN® (Chemical Industry Notes) contains bibliographic and abstract information from journals, trade magazines and newspapers.

CAOLD supplements the CA file with approximately 700 000 records from 1957 to 1966 and provides CAS registry numbers and CA reference numbers to the printed Chemical Abstracts reference.

[STN International, c/o Chemical Abstracts Service, 2540 Olentangy River Road, PO Box 3012, Columbus, OH 43210-0012, USA]

5.5.5 Institute for Scientific Information (ISI) abstracts

Current Chemical Reactions Database. A database of approximately 28 000 reactions per year. Structures are searchable and depict stereochemistry; atom-atom mapping and indication of the reacting centres is also shown diagrammatically. Experimental conditions and yields are given in addition to bibliographic data.

The Chemistry Citation Index. This is a CD-ROM database of abstracts, updated every month. It is searchable by abstract and cited references allowing practical rapid access to relevant articles and citations.

Index Chemicus Database. Abstracted from leading international journals this database contains recently reported novel compounds represented by 2D-structures with stereochemistry. Structure searching is available in addition to searches by formula, molecular weight, compound category, biological activity and comments.

Four subsets are available: Pharmaceutical Compounds (80 000), Agrochemical Compounds (15 000), Biologically Active Compounds (20 000) and Synthetic Intermediates (12 000).

Current Contents. Available in a 'Physical, Chemical and Earth Sciences' edition, this weekly CD-ROM product reproduces tables of contents from leading journals, along with abstracts, author and keyword information.

[Institute for Scientific Information, 3501 Market Street, Philadelphia, PA 19104, USA]

5.5.6 *Crossfire* from the Beilstein Institute

This provides access to the entire Beilstein structure file (some 6 000 000 connection tables) and related information, and is available on IBM RISC 6000 workstations. Structures, Beilstein registry number, CAS registry numbers and field availability may be browsed in-house prior to on-line access of the factual data.

[Beilstein Informationssysteme GmbH, Varrentrappstrasse 40-42, D-60486, Frankfurt].

6 Patent literature

A patent is a legal document in which an inventor discloses to the public the technical content of an invention. The inventor gives up the secrecy of his/her invention in return for a monopoly for a specified period.

Each country issues its own patents. A patent is valid only in the country in which it is issued and so the same invention is usually patented in several countries. These patent duplications are known as equivalents.

Before a patent is granted, the patent application is examined for novelty, invention and utility. This examination is a time-consuming process and many countries (e.g. the UK, Japan and Germany) now publish unexamined patent applications, thus shortening the time to publication. Other countries publish only issued patents.

Patent documents are also issued by the European Patent Office (European Patents) and by the International Bureau of the World Intellectual Property Organization (WIPO) under the Patent Cooperation Treaty (PCT) (the so-called World Patents).

The European Patent Office (EPO) was set up by certain European countries (EC and others) following a convention in 1973. The EPO grants patents that are valid in whichever countries are designated. European patent documents are published in English, French or German, with the claims translated into all three languages.

The Patent Cooperation Treaty set up a system of centralised searching for member states all over the world. The search results are passed on to the member states, who then each decide whether or not to grant the patent. Thus, the PCT itself does not result in a granted patent, but the PCT patent applications are published. These applications may be published in English, French, German, Japanese or Russian, although there is an abstract that is always translated into English.

Patents contain a wealth of technical and scientific information. They are of particular interest in organic chemistry because of the large number of newly synthesised chemical compounds that are reported particularly by the pharmaceutical and agrochemical industries.

Often, patent claims contain Markush formulae, named after a US chemist who was the first to file a patent application containing them. These make it possible to claim an invention for a vast number of compounds, even though few of them will have been prepared in the laboratory. An extreme example of a Markush structure is given in Figure 6.1 (taken from *Chem. Abstr.* 1994, **120**: 8603r). The symbols R^1, R^2, R^3, R^4, R^5, A, X, *m* and *n* each represent number of choices, and so their combination gives rise to a large number of possible compounds; in this particular case, an infinite number is possible because some of the substituents have open-ended descriptions.

Many chemists will first encounter patents when searching *Chemical Abstracts* (CA), which covers patents from 27 nations and European and World Patents. In CA, patents are integrated with other literature, and so a search of CA will often lead to patent references. Where an invention is patented in more than one country, CA abstracts the first patent it receives (the basic patent); the subsequent patents on the same invention (the equivalent patents) are not abstracted but are cross-referenced to the basic patent in the Patent Index. Thus, for example, if a CA reference to a Japanese patent is retrieved, the Patent Index can be used to check whether there is an equivalent patent in English (e.g. a British or US patent).

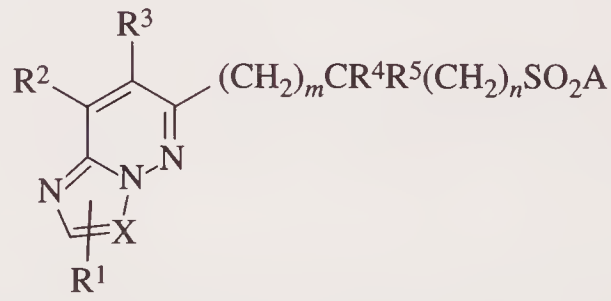


Figure 6.1 An extreme example of a Markush formula. X = CH, or N; R^1 = H, or (substituted) lower alkyl, or halo; R^2, R^3 = H, or (substituted) lower alkyl, or R^2R^3 form a five- to seven-membered ring fused to the pyridazine ring; R^4, R^5 = H, or (substituted) lower alkyl, or R^4R^5 form a three- to seven-membered homocyclic or heterocyclic ring containing adjacent carbon atoms; A = (substituted) amine; *m*, *n* = 1–4.

A substance from a patent is only selected for inclusion in the CA Chemical Substance Index when there is firm evidence in the patent that the substance has actually been prepared or when the substance is unambiguously defined in the patent claims. No attempt is made to index all possible compounds represented by a Markush formula.

Comprehensive coverage of chemical patents is also provided by Derwent's *Chemical Patent Index* (CPI), which is available online on several hosts.

7 Nomenclature in *Chemical Abstracts*

7.1 Introduction

The chemical nomenclature used in *Chemical Abstracts* (CA) Indexes has developed in parallel and generally in accordance with the rules published by the International Union of Pure and Applied Chemistry (IUPAC). However, in the CA system, each substance is assigned a single, unique name, whereas the IUPAC system often leads to two or more equally acceptable names for the same compound.

A major revision of CA Index Names was carried out in 1972 when the Ninth Collective Index (9CI) period began. The CA Index Names for almost all organic substances have continued unchanged since then, and they are often referred to as 9CI names. This section deals with the assignment of 9CI names for organic compounds.

In order to use CA efficiently, some knowledge of how CA Index Names are derived is essential. Even when a chemist uses the Formula Index, there is usually more than one substance with the desired formula, and the only way to determine whether any of them is the required compound is by examining the name. Especially when dealing with very common formulae, an ability to work out the Index Name is essential. The following is a brief guide to assigning CA Index Names. It is by no means comprehensive and will fail for some types of compounds. However, it is valid for the vast majority.

7.2 CA Index Names

Chemical names appear in CA Indexes in inverted form. For example, the compound 1,3-dichlorobenzene appears as 'Benzene, 1,3-dichloro-'. 'Benzene' is called the heading parent and it is followed by a comma (the comma of inversion) and then the rest of the name.

A CA Index Name may have up to four components: heading parent, substituent, modification and stereochemistry. All substances have a heading parent, but one or more of the other parts may not be present for any particular compound. As an example, we shall consider the following Index Name:

2-Butenoic acid, 3-amino-, ethyl ester, (*Z*)-

- The **heading parent** is '2-Butenoic acid'. This forms the basis for the alphabetisation of the index. To look up a compound in the CA Substance Indexes, you must be able to decide which portion of the molecule represents the parent.
- The **substituent** is '3-amino-'. In the indexes, substituents follow a boldfaced dash and the comma of inversion.
- The **modification** is 'ethyl ester'. The modification, as its name suggests, modifies the principal functional group in the compound. For example, it is used for anhydrides, esters and salts of acids, oxides, sulfides and selenides of ring systems containing P and As, hydrazones and oximes of aldehydes and ketones, and hydrochlorides and other salts of amines. These modified groups have the same standing in the order of precedence (see below) as the unmodified groups. Note that in the case of esters, reinversion is allowed so that, for example, 'Ethyl acetate' is a correct name for 'Acetic acid, ethyl ester'.
- The **stereochemistry** is '(*Z*)-'.

7.2.1 Heading parent

The heading parent consists of two parts: a *molecular skeleton* and a *suffix expressing the principal functional group*, together with any necessary locants. In our example, '2-Butene' is the molecular skeleton and '-oic acid' is the functional suffix; the '-e' at the end of butene is elided when the suffix is added. For compounds with no functional groups, the heading parent consists solely of a molecular skeleton name, e.g. Methane, Pyridine.

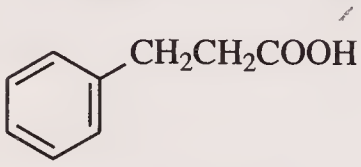
(*a*) Molecular skeleton

The main types of molecular skeleton are:

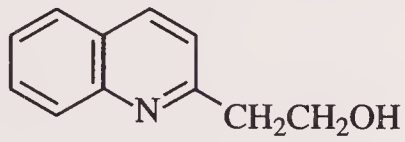
- Unbranched chains of carbon atoms, with or without multiple bonds; e.g. methane, ethane, propane,

butane, pentane, etc., and unsaturated analogues such as 1-butene, 1,3-pentadiyne.

- Rings or ring systems; e.g. cyclopentane, benzene, pyridine, benzo[*b*]thiophene.
- Conjunctive parents (see Chapter 8, under *conjunctive nomenclature*). A conjunctive name may be applied when the principal functional group is attached to a saturated carbon chain that is directly attached to a cyclic component by a carbon–carbon single bond. For example:



benzenepropanoic acid



2-quinoline ethanol

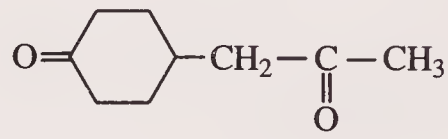
(*b*) Principal functional groups

The principal functional group in a compound is that group which appears nearest the top in Table 7.1.

(*c*) Sequence rules for choosing the heading parent

The first step in choosing the index heading parent is to identify the principal functional group. The second step is to identify the molecular skeleton to which the principal functional group is attached. For many compounds, this will cause no problems. For example, in $H_2NCH_2CH_2OH$, the alcohol function takes precedence over the amine, and the heading parent is 'Ethanol'. In other compounds, a choice of molecular skeletons is possible.

Consider the following compound:



This contains two ketone groups, which cannot be expressed in a single parent. The heading parent could either be 'Cyclohexanone' or '2-Propanone'. In order to determine which it is, certain rules are applied in sequence until a decision is reached. These

Table 7.1 Functional groups in order of priority

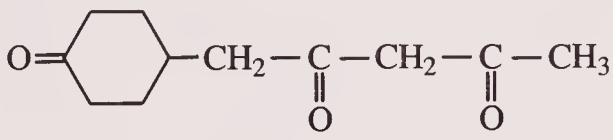
Functional group		Suffix[a]	Prefix[a]
cations (e.g. ammonium)	e.g. $>N^+<$	-ium	
carboxylic acid	–COOH	-oic acid or -carboxylic acid[b]	carboxy
sulfonic acid	$–SO_3H$	-sulfonic acid	sulfo
carboxylic acid halide	–COX	-oyl halide or -carbonyl halide[b]	(haloformyl)
sulfonyl halide	$–SO_2X$	-sulfonyl halide	(halosulfonyl)
carboxamide	$–CONH_2$	-amide or -carboxamide[b]	(aminocarbonyl)
sulfonamide	$–SO_2NH_2$	-sulfonamide	(aminosulfonyl)
nitrile	–CN	-nitrile or -carbonitrile[b]	cyano
aldehyde	–CHO	-al or -carboxaldehyde[b]	formyl
ketone	=O	-one	oxo
thione	=S	-thione	thioxo
alcohol and phenol	–OH	-ol	hydroxy
thiol	–SH	-thiol	mercapto
amine	$–NH_2$	-amine	amino
imine	=NH	-imine	imino

[a] Only one type of function may be expressed as a suffix in a name. If more than one type of functional group is present, those of lower priority are expressed using substituent prefixes.

[b] The suffixes '-oic acid', '-oyl chloride', '-amide', '-nitrile' and '-al' are used when the functional group is at the end of a carbon chain, as in pentanoic acid. The endings '-carboxylic acid', etc., are used when the group is attached to a ring, as in 2-pyridinecarboxylic acid.

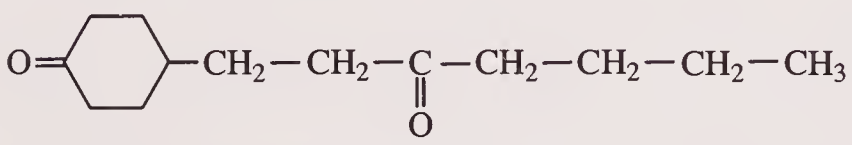
rules are as follows:

1. The preferred parent is that which expresses the maximum number of the principal functional group.



'2,4-Pentanedione' (which expresses two ketone groups) is preferred over 'Cyclohexanone' (which expresses only one ketone group). The Index Name is '2,4-Pentanedione, 1-(4-oxocyclohexyl)-'.

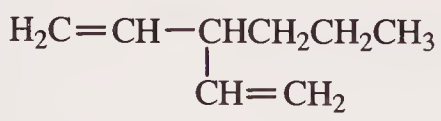
2. A cyclic molecular skeleton is preferred to an acyclic carbon chain.



'Cyclohexanone' (with a cyclic skeleton) is preferred to '3-Heptanone' (with an acyclic skeleton). The Index Name is 'Cyclohexanone, 4-(3-oxoheptyl)-'.

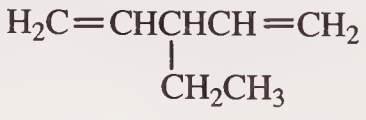
3. The preferred parent contains the senior ring system. For ring systems, nitrogen heterocycles > other heterocycles > carbocycles (here > means is/are preferred to). Thus, pyridine > furan > naphthalene. If two ring systems are of a type, then that with the greater number of individual rings is preferred; e.g. quinoline > pyridine, and naphthalene > benzene. A further 12 more criteria are needed to allow a decision to be made in all cases. These can be found in the CA Index Guide, Appendix IV, paragraph 138.

4. The preferred parent is that which contains the maximum possible number of skeletal atoms.



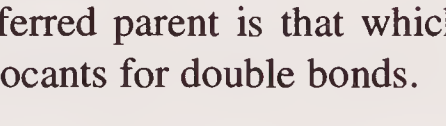
'1-Hexene' (six atoms) is preferred to '1,4-Pentadiene' (five atoms). The Index Name is '1-Hexene, 3-ethenyl-'.

5. For acyclic parents, that parent which expresses the maximum number of multiple bonds (double or triple) is preferred.



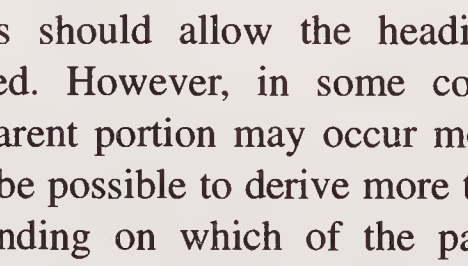
'1,4-Pentadiene' (two multiple bonds) is preferred to '1-Pentene' (one multiple bond). The Index Name is '1,4-Pentadiene, 3-ethyl-'.

6. If a decision has not yet been made, then, for acyclic parents, double bonds are preferred to triple bonds.



'1,4-Pentadiene' (two double bonds) is preferred to '1-Penten-4-yne' (one double bond). The Index Name is '1,4-Pentadiene, 3-ethynyl-'.

7. The preferred parent is that which contains the lowest locants for functional groups.

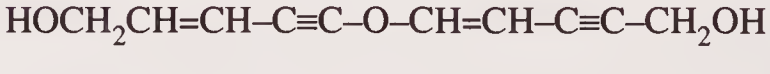


'1,2-Benzenediol' (locants 1,2) is preferred to '1,3-Benzenediol' (locants 1,3). The Index Name is '1,2-Benzenediol, 3-[(2,4-dihydroxyphenyl)methyl]-'.

8. The preferred parent is that which contains the lowest locants for multiple bonds (double or triple).

'2-Butyn-1-ol' (multiple-bond locant 2) is preferred to '3-Buten-1-ol' (multiple-bond locant 3). The Index Name is '2-Butyn-1-ol, 4-[(4-hydroxy-1-butenyl)oxy]-'.

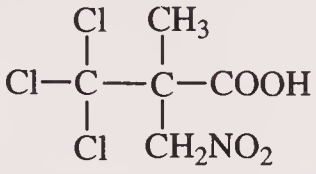
9. The preferred parent is that which contains the lowest locants for double bonds.



'2-Penten-4-yn-1-ol' (double-bond locant 2) is preferred to '4-Penten-2-yn-1-ol' (double-bond locant 4). The Index Name is '2-Penten-4-yn-1-ol, 5-[(5-hydroxy-1-penten-3-ynyl)oxy]-'.

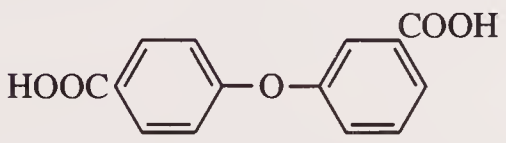
These rules should allow the heading parent to be identified. However, in some compounds the preferred parent portion may occur more than once and it may be possible to derive more than one valid name depending on which of the parent portions is chosen. A few more rules are needed to allow a unique Index Name to be chosen.

10. The Index Name is based on that heading parent to which is attached the greatest number of substituents.



'Propanoic acid' is the parent, but three different names are possible. The Index Name is 'Propanoic acid, 3,3,3-trichloro-2-methyl-2-(nitromethyl)-' (five substituents on the propanoic acid parent), which is preferred to 'Propanoic acid, 2-methyl-3-nitro-2-(trichloromethyl)-' (three substituents attached to the parent propanoic acid) and 'Propanoic acid, 2-(nitromethyl)-2-(trichloromethyl)-' (two substituents on the propanoic acid parent).

11. The Index Name is based on that heading parent which gives the lowest locants for substituents.

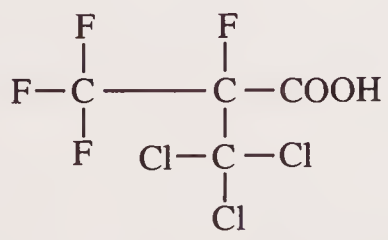


Two 'Benzoic acid' moieties are present. The Index Name is 'Benzoic acid, 3-(4-carboxyphenoxy)-' (substituent at the 3 position on the parent benzoic acid), which is preferred to 'Benzoic acid, 4-(3-carboxyphenoxy)-' (substituent at the 4 position on the parent benzoic acid).

12. If no decision has been made at this point, a multiplicative name may be possible (see section 8.2 under **multiplicative nomenclature**).

The Index Name is 'Ethanol, 2,2′-iminobis-'.

13. If all else fails, the CA Index Name is that one which will appear first in the CA Substance Index.



The two possible Index Name are: 'Propanoic acid, 2,3,3,3-tetrafluoro-2-(trichloromethyl)-' and 'Propanoic acid, 3,3,3-trichloro-2-fluoro-2-(trifluoromethyl)-'. The first name is the Index Name, since this would appear first alphabetically in the CA Substance Index (tetrafluoro comes before trichloro).

(*d*) Non-functional groups

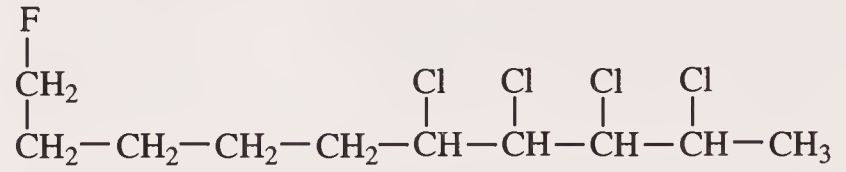
Some groups are considered to be non-functional and are always cited as substituents. These include the groups shown in Table 7.2.

7.2.2 Substituents

(*a*) Numbering of substituents

If a molecular skeleton can be numbered in more than one way, then it should be numbered in such a way so as *to give the substituents the lowest set of locants*. The locants for all the substituents (regardless of what the substituents are) are arranged in numerical order; the possible sets of locants are then compared *number by number* until a difference is found.

For example, consider the following:



This is 'Decane, 6,7,8,9-tetrachloro-1-fluoro-' not 'Decane, 2,3,4,5-tetrachloro-10-fluoro-'; in the first name the substituents have the locants 1,6,7,8,9, and in the second name 2,3,4,5,10.

Table 7.2 Non-functional groups cited as substituents

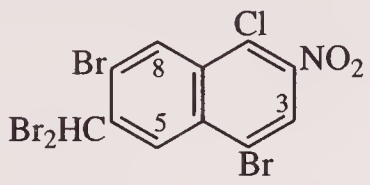
bromo-	–Br
chloro-	–Cl
fluoro-	–F
iodo-	–I
nitroso-	–NO
nitro-	$-NO_2$
isocyano-	–NC
isocyanato-	–NCO
diazo-	$=N_2$
azido-	$-N_3$
ether (R-oxy)[a]	–OR
sulfide (R-thio)[a]	–SR
sulfoxide (R-sulfinyl)[a]	–S(O)R
sulfone (R-sulfonyl)[a]	$-S(O)_2R$

[a] For example, (cyclopentyloxy), (cyclopentylthio), etc., when R = cyclopentyl.

(*b*) Alphabetisation of substituents

Substituent prefixes are placed in alphabetical order according to their name; *only then are numerical prefixes (di-, tri-, etc.) placed in front of each as required* and the locants inserted.

For example, consider:



The substituents are: 1-chloro-, 2-nitro-, 4-bromo-, 6-(dibromomethyl)- and 7-bromo-. The substituents are cited in alphabetical order, i.e. bromo, then chloro, then (dibromomethyl), then nitro. The Index Name is 'Naphthalene, 4,7-dibromo-1-chloro-6-(dibromomethyl)-2-nitro-'.

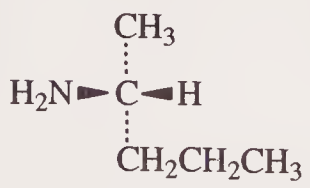
(Dibromomethyl) is an example of a complex substituent, one that is made up of two or more simple substituents. A complex substituent requires enclosing parentheses, and is alphabetised at its first letter, regardless of the origin of this letter, e.g. 'b' from '(bromomethyl)', 'd' from '(dibromomethyl)' and 't' from '(tribromomethyl)'.

7.2.3 Stereochemistry and stereochemical descriptors

The following is a very brief summary of the representation and description of simple stereochemistry with special reference to the *Dictionary of Organic Compounds* and *Chemical Abstracts*. See also the relevant entries in Chapter 8, especially under *amino acids*, *carbohydrates*, D-, *R*- and *sequence rule*.

(*a*) Simple compounds with one chiral centre

Where the absolute configuration is known, the compound is illustrated in DOC 6 using the standard Fischer-type drawing, and following the convention that the principal chain occupies the vertical position, with the head of the chain uppermost.



(*R*)-form

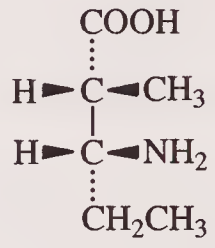
2-pentylamine

The enantiomer illustrated is normally the first one described in the entry ((*R*)- if both are described), except in the case of the common protein amino acids, where in most cases the (*S*)-form is the common one and to illustrate the (*R*)-form would be confusing. The alternative D- or L-descriptor is given in addition for such compounds.

CA practice is similar, except that D/L-descriptors are used for the common amino acids (the CAS Name also remains the amino acid name, e.g. alanine not 2-aminopropanoic acid).

(*b*) Compounds with two chiral centres

The same conventions are followed, with the (*R*,*R*)-isomer (if documented) being illustrated and presented first in the entry.



(2*R*,3*R*)-form

3-amino-2-methylpentanoic acid

For the racemates, the symbols (2*RS*,3*RS*) and (2*RS*,3*SR*) are used. In the (now relatively few) cases where the absolute configuration appears still to be unknown, asterisked symbols, e.g. (2*R**,3*R**) and (2*R**,3*S**), are used.

CA presentation is different. The relative stereochemistry is first indicated using the *R**,*S** labels. *R** *is allocated to the centre of highest sequence priority*, e.g. in the above example, position 3. The general descriptor (*R**,*S**) for this diastereoisomer is then modified where the absolute configuration is known, and the citation refers to the optically active material. Thus the isomer illustrated above is [*S*-(*R**,*S**)]* and its racemate, when specifically referred to, is [(*R**,*S**)-(±)]. (This illustrates an important source of 'other CAS Registry Numbers' in a DOC entry. (*R**,*S**) and [(*R**,*S**)-(±)] will each have a Registry Number: the general Registry Number for (*R**,*S**) cannot readily be fitted to the DOC entry structure.)

(*c*) Cyclic structures

The application of the above principles to simple cyclic structures is straightforward. For the use of the sequence rule in symmetrical cases such as 1,4-cyclohexanediol, see Chapter 8 under *sequence rule*.

In the case of cyclic structures with several substituents (e.g. cyclitols), the (α,β)-convention is clearer and unambiguous. The symbols *r* and *s* denoting the configurations of pseudoasymmetric centre are not used in DOC.

Beilstein uses a number of additional stereochemical descriptors for specialised situations. Examples are (*RS*), R_a, S_a and Ξ. For full details, see the booklet *Stereochemical Conventions in the Beilstein Handbook of Organic Chemistry* available free from the Beilstein Institute (see Section 5.3 for address).

7.3 Older names encountered in CA

Major changes to *Chemical Abstracts* index nomenclature were made at the beginning of 1972 at the changeover from the 8th Collective Index (8CI) to the 9th Collective Index (9CI). The use of many trivial names was discontinued. The following list equates current 9CI names with the trivial names that were used in 8CI (and earlier indexes). An asterisk (*) indicates that the trivial name was used in 8CI for the unsubstituted substance only; substituted derivatives were indexed elsewhere (see the *8CI Index Guide*). For benzenamine derivatives, '*ar*-' indicates that substitution is on the benzene ring and not on the amine nitrogen atom. For piperidine derivatives, '*C*-' indicates that substitution is on a carbon atom and not on the nitrogen atom.

In DOC 6, appropriate names are suffixed 9CI or 8CI, but names used in CA before 8CI are not specially labelled.

8CI Name	9CI Name
Acetamidine	Ethanimidamide
Acetanilide	Acetamide, *N*-phenyl-
Acetanisidide	Acetamide, *N*-(methoxyphenyl)-
Acetoacetic acid	Butanoic acid, 3-oxo-
Acetonaphthone	Ethanone, 1-(naphthalenyl)-
Acetone*	2-Propanone
Acetophenetidide	Acetamide, *N*-(ethoxyphenyl)-
Acetophenone	Ethanone, 1-phenyl-
Acetotoluidide	Acetamide, *N*-(methylphenyl)-
Acetoxylidide	Acetamide, *N*-(dimethylphenyl)-
Acetylene	Ethyne
Acrolein	2-Propenal
Acrylic acid	2-Propenoic acid
Adamantane	Tricyclo[3.3.1.1^{3,7}]decane
Adipic acid*	Hexanedioic acid
Allene*	1,2-Propadiene
Alloxan	2,4,5,6(1*H*,3*H*)-Pyrimidinetetrone
Alloxazine	Benzo[*g*]pteridine-2,4(1*H*,3*H*)-dione
Allyl alcohol*	2-Propen-1-ol
Allylamine	2-Propen-1-amine
Aniline	Benzenamine
Anisic acid	Benzoic acid, methoxy-
Anisidine	Benzenamine, *ar*-methoxy-
Anisole	Benzene, methoxy-
Anthranilic acid	Benzoic acid, 2-amino-
Anthraquinone	9,10-Anthracenedione
Anthroic acid	Anthracenecarboxylic acid
Anthrol	Anthracenol
Anthrone	9(10*H*)-Anthracenone
Atropic acid	Benzeneacetic acid, α-methylene-
Azelaic acid*	Nonanedioic acid
Azobenzene	Diazene, diphenyl-
Azoxybenzene	Diazene, diphenyl-, 1-oxide
Barbituric acid	2,4,6(1*H*,3*H*,5*H*)-Pyrimidinetrione
Benzanilide	Benzamide, *N*-phenyl-
Benzhydrol	Benzenemethanol, α-phenyl-
Benzidine	(1,1′-Biphenyl)-4,4′-diamine
Benzil	Ethanedione, diphenyl-
Benzilic acid	Benzeneacetic acid, α-hydroxy-α-phenyl-
Benzoin	Ethanone, 2-hydroxy-1,2-diphenyl-
Benzophenone	Methanone, diphenyl-
o-Benzoquinone	3,5-Cyclohexadiene-1,2-dione
p-Benzoquinone	2,5-Cyclohexadiene-1,4-dione
Benzyl alcohol	Benzenemethanol
Benzylamine	Benzenemethanamine
Bibenzyl	Benzene, 1,1′-(1,2-ethanediyl)-bis-
Bornane	Bicyclo[2.2.1]heptane, 1,7,7-trimethyl-
Butyl alcohol*	1-Butanol
sec-Butyl alcohol*	2-Butanol
tert-Butyl alcohol*	2-Propanol, 2-methyl-
Butylamine	1-Butanamine
Butyraldehyde	Butanal

Butyric acid	Butanoic acid
Butyrophenone	1-Butanone, 1-phenyl-
Caffeine	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
Camphene*	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-
Camphor*	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-
Carane	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-
Carbodiimide	Methanediimine
Carbostyril	2(1*H*)-Quinolinone
Carvacrol	Phenol, 2-methyl-5-(1-methylethyl)-
Chalcone	2-Propen-1-one, 1,3-diphenyl-
Chroman	2*H*-1-Benzopyran, 3,4-dihydro-
Chromone	4*H*-1-Benzopyran-4-one
Cinchoninic acid	4-Quinolinecarboxylic acid
Cinnamic acid	2-Propenoic acid, 3-phenyl-
Cinnamyl alcohol*	2-Propen-1-ol, 3-phenyl-
Citraconic acid*	2-Butenedioic acid, 2-methyl-, (*Z*)-
Citric acid	1,2,3-Propanetricarboxylic acid, 2-hydroxy-
Coumarin	2*H*-1-Benzopyran-2-one
Cresol	Phenol, methyl-
Cresotic acid	Benzoic acid, hydroxymethyl-
Crotonic acid	2-Butenoic acid
Cumene	Benzene, (1-methylethyl)-
Cumidine	Benzenamine, 4-(1-methylethyl)-
Cymene	Benzene, methyl(1-methylethyl)-
Cytosine	2(1*H*)-Pyrimidinone, 4-amino-
Diacetamide	Acetamide, *N*-acetyl-
Dibenzamide	Benzamide, *N*-benzoyl-
Diethylamine	Ethanamine, *N*-ethyl-
Diethylene glycol*	Ethanol, 2,2′-oxybis-
Diimide	Diazene
Dimethylamine	Methanamine, *N*-methyl-
Divicine	4,5-Pyrimidinedione, 2,6-diamino-1,6-dihydro-
Elaidic acid	9-Octadecenoic acid, (*E*)-
Elaidolinolenic acid	9,12,15-Octadecatrienoic acid, (*E*,*E*,*E*)-
Ethyl alcohol*	Ethanol
Ethyl ether*	Ethane, 1,1′-oxybis-
Ethyl sulfide*	Ethane, 1,1′-thiobis-
Ethylamine	Ethanamine
Ethylene	Ethene
Ethylene glycol*	1,2-Ethanediol
Ethylene oxide*	Oxirane
Ethylenimine*	Aziridine
Flavan	2*H*-1-Benzopyran, 3,4-dihydro-2-phenyl-
Flavanone	4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Flavone	4*H*-1-Benzopyran-4-one, 2-phenyl-
Flavylium	1-Benzopyrylium, 2-phenyl-
Fulvene*	1,3-Cyclopentadiene, 5-methylene-
Fumaric acid	2-Butenedioic acid, (*E*)-
2-Furaldehyde	2-Furancarboxaldehyde
Furfuryl alcohol	2-Furanmethanol
Furfurylamine	2-Furanmethanamine
Furoic acid	Furancarboxylic acid
Gallic acid	Benzoic acid, 3,4,5-trihydroxy-
Gentisic acid	Benzoic acid, 2,5-dihydroxy-
Glutaconic acid	2-Pentenedioic acid
Glutaric acid	Pentanedioic acid
Glyceraldehyde	Propanal, 2,3-dihydroxy-
Glyceric acid	Propanoic acid, 2,3-dihydroxy-
Glycerol*	1,2,3-Propanetriol
Glycidic acid	Oxiranecarboxylic acid
Glycolic acid	Acetic acid, hydroxy-
Glyoxal	Ethanedial
Glyoxylic acid	Acetic acid, oxo-
Guanine	6*H*-Purin-6-one, 2-amino-1,7-dihydro-
Heteroxanthine	1*H*-Purine-2,6-dione, 3,7-dihydro-7-methyl-
Hippuric acid	Glycine, *N*-benzoyl-
Hydantoin	2,4-Imidazolidinedione
Hydracrylic acid	Propanoic acid, 3-hydroxy-
Hydratropic acid	Benzeneacetic acid, α-methyl-
Hydrazobenzene	Hydrazine, 1,2-diphenyl-
Hydrocinnamic acid	Benzenepropanoic acid
Hydrocoumarin	2*H*-1-Benzopyran-2-one, 3,4-dihydro-
Hydroorotic acid	4-Pyrimidinecarboxylic acid, hexahydro-2,6-dioxo-
Hydroquinone	1,4-Benzenediol
Hydrouracil	2,4(1*H*,3*H*)-Pyrimidinedione, dihydro-

Hypoxanthine	6*H*-Purin-6-one, 1,7-dihydro-
Indan	1*H*-Indene, 2,3-dihydro-
Indoline	1*H*-Indole, 2,3-dihydro-
Indone	1*H*-Inden-1-one
Isobarbituric acid	2,4,5(3*H*)-Pyrimidinetrione, dihydro-
Isobutyl alcohol*	1-Propanol, 2-methyl-
Isobutyric acid*	Propanoic acid, 2-methyl-
Isocaffeine	1*H*-Purine-2,6-dione, 3,9-dihydro-1,3,9-trimethyl-
Isocarbostyril	1(2*H*)-Isoquinolinone
Isochroman	1*H*-2-Benzopyran, 3,4-dihydro-
Isocoumarin	1*H*-2-Benzopyran-1-one
Isocytosine*	4(1*H*)-Pyrimidinone, 2-amino-
Isoflavan	2*H*-1-Benzopyran, 3,4-dihydro-3-phenyl-
Isoflavanone	4*H*-1-Benzopyran-4-one, 2,3-dihydro-3-phenyl-
Isoflavone	4*H*-1-Benzopyran-4-one, 3-phenyl-
Isoflavylium	1-Benzopyrylium, 3-phenyl-
Isoguanine	2*H*-Purin-2-one, 6-amino-1,3-dihydro-
Isohexyl alcohol*	1-Pentanol, 4-methyl-
Isoindoline	1*H*-Isoindole, 2,3-dihydro-
Isonicotinic acid	4-Pyridinecarboxylic acid
Isonipecotic acid	4-Piperidinecarboxylic acid
Isopentyl alcohol*	1-Butanol, 3-methyl-
Isophthalic acid	1,3-Benzenedicarboxylic acid
Isoprene*	1,3-Butadiene, 2-methyl-
Isopropyl alcohol*	2-Propanol
Isopropylamine	2-Propanamine
Isoquinaldic acid	1-Isoquinolinecarboxylic acid
Isovaleric acid*	Butanoic acid, 3-methyl-
Ketene	Ethenone
Lactic acid	Propanoic acid, 2-hydroxy-
Lauric acid*	Dodecanoic acid
Lepidine	Quinoline, 4-methyl-
Levulinic acid	Pentanoic acid, 4-oxo-
Linoleic acid	9,12-Octadecadienoic acid, (*Z*,*Z*)-
Linolelaidic acid	9,12-Octadecadienoic acid, (*E*,*E*)-
Linolenic acid	9,12,15-Octadecatrienoic acid, (*Z*,*Z*,*Z*)-
γ-Linolenic acid	6,9,12-Octadecatrienoic acid, (*Z*,*Z*,*Z*)-
Lumazine	2,4(1*H*,3*H*)-Pteridinedione
Lupetidine*	Piperidine, *C*,*C*′-dimethyl-
Lutidine	Pyridine, dimethyl-
Maleic acid	2-Butenedioic acid, (*Z*)-
Maleic anhydride	2,5-Furandione
Maleimide	1*H*-Pyrrole-2,5-dione
Malic acid	Butanedioic acid, hydroxy-
Malonic acid	Propanedioic acid
Mandelic acid	Benzeneacetic acid, α-hydroxy-
Melamine	1,3,5-Triazine-2,4,6-triamine
Menthane	Cyclohexane, methyl(1-methylethyl)-
Mesaconic acid*	2-Butenedioic acid, 2-methyl-, (*E*)-
Mesitol	Phenol, 2,4,6-trimethyl-
Mesitylene	Benzene, 1,3,5-trimethyl-
Mesoxalic acid	Propanedioic acid, oxo-
Metanilic acid	Benzenesulfonic acid, 3-amino-
Methacrylic acid*	2-Propenoic acid, 2-methyl-
Methyl sulfoxide*	Methane, sulfinylbis-
Methylamine	Methanamine
Methylenimine	Methanimine
Myristic acid*	Tetradecanoic acid
Naphthalic acid	1,8-Naphthalenedicarboxylic acid
Naphthoic acid	Naphthalenecarboxylic acid
Naphthol	Naphthalenol
Naphthoquinone	Naphthalenedione
Naphthylamine	Naphthalenamine
Nicotinic acid	3-Pyridinecarboxylic acid
Nipecotic acid	3-Piperidinecarboxylic acid
Norbornane	Bicyclo[2.2.1]heptane
Norcarane	Bicyclo[4.1.0]heptane
Norpinane	Bicyclo[3.1.1]heptane
Oleic acid	9-Octadecenoic acid, (*Z*)-
Orotic acid	4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-
Oxalacetic acid	Butanedioic acid, oxo-
Oxalic acid	Ethanedioic acid
Palmitic acid*	Hexadecanoic acid
Paraxanthine	1*H*-Purine-2,6-dione, 3,7-dihydro-1,7-dimethyl-
Pentaerythritol*	1,3-Propanediol, 2,2-bis-(hydroxymethyl)-

Pentyl alcohol*	1-Pentanol
tert-Pentyl alcohol*	2-Butanol, 2-methyl-
Peroxyacetic acid	Ethaneperoxoic acid
Peroxybenzoic acid	Benzenecarboperoxoic acid
Phenethyl alcohol	Benzeneethanol
Phenethylamine	Benzeneethanamine
Phenetidine	Benzenamine, *ar*-ethoxy-
Phenetole	Benzene, ethoxy-
Phenylenediamine	Benzenediamine
Phloroglucinol	1,3,5-Benzenetriol
Phthalan	Isobenzofuran, 1,3-dihydro-
Phthalic acid	1,2-Benzenedicarboxylic acid
Phthalic anhydride	1,3-Isobenzofurandione
Phthalide	1(3*H*)-Isobenzofuranone
Phthalimide	1*H*-Isoindole-1,3(2*H*)-dione
Phthalonic acid	Benzeneacetic acid, 2-carboxy-α-oxo-
Phytol	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-
Picoline	Pyridine, methyl-
Picolinic acid	2-Pyridinecarboxylic acid
Picric acid	Phenol, 2,4,6-trinitro-
Pimelic acid*	Heptanedioic acid
Pinane	Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-
Pipecolic acid	2-Piperidinecarboxylic acid
Pipecoline	Piperidine, *C*-methyl-
Piperonal	1,3-Benzodioxole-5-carboxaldehyde
Piperonylic acid	1,3-Benzodioxole-5-carboxylic acid
Pivalic acid*	Propanoic acid, 2,2-dimethyl-
Propiolic acid	2-Propynoic acid
Propionaldehyde	Propanal
Propionic acid	Propanoic acid
Propionitrile	Propanenitrile
Propiophenone	1-Propanone, 1-phenyl-
Propyl alcohol*	1-Propanol
Propylamine	1-Propanamine
Propylene oxide	Oxirane, methyl-
Protocatechuic acid	Benzoic acid, 3,4-dihydroxy-
Pyridone	Pyridinone
Pyrocatechol	1,2-Benzenediol
o-Pyrocatechuic acid	Benzoic acid, 2,3-dihydroxy-
Pyrogallol	1,2,3-Benzenetriol
Pyruvic acid	Propanoic acid, 2-oxo-
Quinaldic acid	2-Quinolinecarboxylic acid
Quinaldine	Quinoline, 2-methyl-
Quinolone	Quinolinone
Quinuclidine	1-Azabicyclo[2.2.2]octane
Resorcinol	1,3-Benzenediol
α-Resorcylic acid	Benzoic acid, 3,5-dihydroxy-
β-Resorcylic acid	Benzoic acid, 2,4-dihydroxy-
γ-Resorcylic acid	Benzoic acid, 2,6-dihydroxy-
Ricinelaidic acid	9-Octadecenoic acid, 12-hydroxy-, [*R*-(*E*)]-
Ricinoleic acid	9-Octadecenoic acid, 12-hydroxy-, [*R*-(*Z*)]-
Salicylic acid	Benzoic acid, 2-hydroxy-
Sarcosine	Glycine, *N*-methyl-
Sebacic acid*	Decanedioic acid
Sorbic acid	2,4-Hexadienoic acid
Stearic acid*	Octadecanoic acid
Stilbene	Benzene, 1,1′-(1,2-ethenediyl)-bis-
Styrene	Benzene, ethenyl-
Suberic acid*	Octanedioic acid
Succinic acid	Butanedioic acid
Succinic anhydride	2,5-Furandione, dihydro-
Succinimide	2,5-Pyrrolidinedione
Sulfanilic acid	Benzenesulfonic acid, 4-amino-
Tartaric acid	Butanedioic acid, 2,3-dihydroxy-
Tartronic acid	Propanedioic acid, hydroxy-
Taurine	Ethanesulfonic acid, 2-amino-
Terephthalic acid	1,4-Benzenedicarboxylic acid
Tetrolic acid	2-Butynoic acid
Theobromine	1*H*-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-
Theophylline	1*H*-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-
Thujane	Bicyclo[3.1.0]hexane, 4-methyl-1-(1-methylethyl)-
Thymine	2,4(1*H*,3*H*)-Pyrimidinedione, 5-methyl-
Thymol	Phenol, 5-methyl-2-(1-methylethyl)-
Toluene	Benzene, methyl-
Toluic acid	Benzoic acid, methyl-
Toluidine	Benzenamine, *ar*-methyl-
Triethylamine	Ethanamine, *N*,*N*-diethyl-
Trimethylamine	Methanamine, *N*,*N*-dimethyl-
Trimethylene oxide*	Oxetane
Tropic acid*	Benzeneacetic acid, α-(hydroxymethyl)-

Tropolone*	2,4,6-Cycloheptatrien-1-one, 2-hydroxy-
Uracil	2,4(1*H*,3*H*)-Pyrimidinedione
Urete	1,3-Diazete
Uretidine	1,3-Diazetidine
Uric acid	1*H*-Purine-2,6,8(3*H*)-trione, 7,9-dihydro-
Valeric acid	Pentanoic acid
Vanillic acid	Benzoic acid, 4-hydroxy-3-methoxy-
Vanillin	Benzaldehyde, 4-hydroxy-3-methoxy-
Veratric acid	Benzoic acid, 3,4-dimethoxy-
o-Veratric acid	Benzoic acid, 2,3-dimethoxy-
Vinyl alcohol*	Ethenol
Xanthine	1*H*-Purine-2,6-dione, 3,7-dihydro-
Xylene	Benzene, dimethyl-
Xylenol	Phenol, dimethyl-
Xylidine	Benzenamine, *ar*,*ar*′-dimethyl-

8 Glossary of terms used in describing organic structures

8.1 Introduction

This glossary lists terms used in organic chemical nomenclature. It is *not* intended to be a guide on how to name organic compounds. Readers interested in learning how to assign names to compounds should consult the books listed in Section 8.1.2.

8.1.1 Items in the glossary

The glossary includes:

- Names and terms currently used in *Chemical Abstracts* or recommended by IUPAC.
- Names and terms that were once used by *Chemical Abstracts* (particularly in the 8th collective period) or were once recommended by IUPAC.
- Other names and terms that might be encountered in the chemical literature.

Entries will be found for:

- A few specific compounds. Entries have not been made for specific organic compounds; these can be found in DOC 6. However, entries have been made for some inorganic compounds (e.g. borane, phosphoric acid), which may be used as parents when naming organic derivatives.
- Substituent prefixes (radicals), e.g. benzhydryl, thexyl. The current *Chemical Abstracts* name is given in each case. Where a *Chemical Abstracts* name is a two-part name, this has been enclosed in parentheses, e.g. (acetylamino).
- Stereochemical descriptors, e.g. *E*-, *anti*-.
- Suffixes, e.g. -carbohydrazidine, -epane.
- Numerical prefixes, e.g. eicosa, dicta.
- Other prefixes, e.g. *abeo*-, benzo.
- Classes of natural products, e.g. carbohydrates, steroids. Various aspects of their nomenclature are included.
- Other class names, e.g. acetals, calixarenes.
- Types of nomenclature, e.g. conjunctive nomenclature, ring fusion names.

8.1.2 Nomenclature – bibliography

The following are the main guides to the nomenclature of organic compounds.

(*a*) **IUPAC**

Nomenclature of Organic Chemistry (Pergamon, Oxford, 1979). Includes Sections A (Hydrocarbons), B (Fundamental heterocyclic systems), C (Characteristic groups containing C, H, O, N, halogen, S, Se and Te), D (Organic compounds containing other elements), E (Stereochemistry), F (General principles for the naming of natural products and related compounds) and H (Isotopically modified compounds).

A Guide to IUPAC Nomenclature of Organic Compounds (Blackwell Scientific, Oxford, 1993). A 182-page softcover volume to be used in conjunction with *Nomenclature of Organic Chemistry.*

Biochemical Nomenclature and Related Documents (Portland Press, London, 1992). Contains about 40 reprints of articles on specific topics originally published as journal articles. Includes items on the nomenclature of amino acids and peptides, carbohydrates, steroids, carotenoids, corrinoids, tetrapyrroles, etc.

References to journal articles giving IUPAC nomenclature rules about specific types of compounds (e.g. steroids, carbohydrates) are given under the relevant entries in the glossary (Section 8.2). Updates to IUPAC rules and conventions are published from time to time in *Chemistry International*, the IUPAC journal published by Blackwell.

(*b*) ***Chemical Abstracts***

Naming and Indexing of Chemical Substances for Chemical Abstracts (Appendix IV) (Chemical Abstracts Service). A comprehensive account of

CA rules for deriving unique names for chemical compounds. It forms Appendix IV of the *Chemical Abstracts* 1992 Index Guide but it is also available as a separate publication.

Chemical Substance Name Selection Manual (Chemical Abstracts Service, 1982). Details how CAS staff assign index names. Three notebooks, three-hole-punched, ca. 2000 pages.

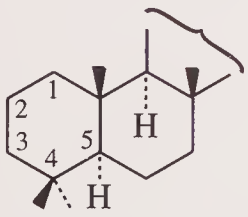
(*c*) **General**

Organic Chemical Nomenclature, P. Fresenius, (Ellis Horwood, Chichester, 1989) Explains the principles and applications of IUPAC rules and compares with alternative systems in current use including WHO, ISO, *Chemical Abstracts*, European Pharmacopoeia and *Beilstein.*

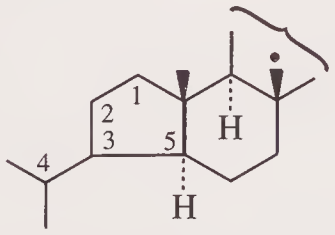
8.2 Glossary

'a' nomenclature See *Replacement nomenclature*

abeo- Used in terpenoid and steroid nomenclature to indicate that a bond has migrated. For example, in a 5(4→3)*abeo*-terpene, the 5–4 bond has been replaced by a 5–3 bond contracting ring A from six to five members. See the *Dictionary of Natural Products* for many examples

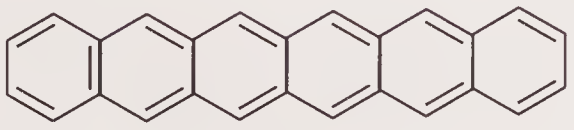


normal triterpene



5(4→3)-*abeo*-triterpene

-acene The names of hydrocarbons containing five or more fused benzene rings in a straight linear arrangement are formed by a numerical prefix followed by -acene



hexacene

acetals Diethers of *gem*-diols $R_2C(OR)_2$ (R can be the same or different). Often named as derivatives of aldehydes or ketones. Thus, acetaldehyde dimethyl acetal is $H_3CCH(OMe)_2$. It is now more usual to name them as dialkoxy compounds, e.g. 1,1-dimethoxyethane. The term 'acetal' is sometimes extended to compounds containing hetero-atoms other than oxygen, as in *N,O*-acetals $R_2C(OR)(NR_2)$. In DOC 6, most acetals are included as derivatives of the aldehyde or ketone. Derivatives of ketones were formerly called ketals, but this term has now been discontinued by IUPAC

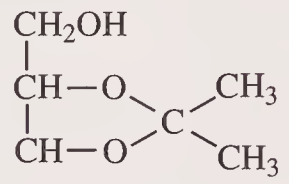
acetamido (acetylamino) $H_3CCONH–$

acetimido This radical name has been used both for (acetylimino) AcN= and for (1-iminoethyl) $H_3CC(=NH)–$

acetimidoyl (1-iminoethyl) $H_3CC(=NH)–$

acetoacetyl (1,3-dioxobutyl) $H_3CCOCH_2CO–$

acetonides Cyclic acetals derived from acetone and diols. Better described as isopropylidene derivatives



glycerol acetonide =
1,2-isopropylidene glycerol

acetonyl (2-oxopropyl) $H_3CCOCH_2–$

acetoxy (acetyloxy) $H_3CCOO–$

acetyl $H_3CCO–$ Often abbreviated to Ac in structural and line formulae. In DOC 6, Ac is used only for acetyl groups attached to heteroatoms

acetylenes A general term for hydrocarbons having one or more triple bonds. 'Alkynes' is now the more usual term. Acetylene itself is HC≡CH

acetylides Metal derivatives of acetylene. Thus, sodium acetylide is HC≡CNa

aci- The acid form of (prefix)

acid anhydrides See *anhydrides*

acid halides See *acyl halides*

***aci*-nitramino** (*aci*-nitroamino) HON(O)=N–

***aci*-nitro** HON(O)= (Methyl-*aci*-nitro) is MeON(O)=. *aci*-Nitro compounds are also known as nitronic acids

acryloyl or **acrylyl** (1-oxo-2-propenyl) $H_2C=CHCO–$

acyl General term for a radical formed from an acid by removal of a hydroxy group, e.g. $H_3CCO–$, $PhSO_2–$. Names for acyl radicals are derived by changing the endings '-ic acid' to '-yl', '-oic acid' to '-oyl', and '-carboxylic acid' to '-carbonyl'

acylals General term for diesters of *gem*-diols. They are named as esters. Thus, $H_3CCH(OAc)_2$ is ethylidene diacetate

acyl halides (acid halides) General term for compounds in which the hydroxy group of an acid is replaced by a halogen atom, e.g. H_3CCOCl, $PhSO_2Br$. They are named by placing the name of the halide after the name of the acyl radical, e.g. acetyl chloride, benzenesulfonyl bromide. In DOC 6, an acid chloride usually appears as a derivative of the acid and is described as the 'chloride'. Other acid halides are treated similarly

acyloins α-hydroxy ketones RCH(OH)COR An acyloin name is formed by changing the '-ic acid' or '-oic acid' of the trivial name of the acid RCOOH to '-oin'. Thus $H_3CCH(OH)COCH_3$ is acetoin. They are now usually given normal substitutive names, e.g. 3-hydroxy-2-butanone

added hydrogen See *H*

additive nomenclature Additive nomenclature involves the addition of an atom or a group of atoms to the structure denoted by the rest of the name. Examples of additive names are: pyridine *N*-oxide, ethylene dibromide and decahydronaphthalene

adipoyl or **adipyl** (1,6-dioxo-1,6-hexanediyl) $–CO(CH_2)_4CO–$

aetio- See *etio-*

aglycones (**aglycons**) Compounds remaining after hydrolysis of the glycosyl groups from glycosides

-al Suffix denoting the aldehyde (–CHO) function when part of an aliphatic chain. Thus, pentanal is $H_3C(CH_2)_3CHO$

alanyl $H_3CCH(NH_2)CO–$ The acyl radical from alanine used in naming peptides

β-alanyl $H_2NCH_2CH_2CO–$ The acyl radical from β-alanine used in naming peptides

alcohols Compounds ROH (R = alkyl). Named using the suffix '-ol', e.g. 2-butanol, or the substituent prefix 'hydroxy'

aldaric acids Dicarboxylic acids formed by oxidation of aldoses at both terminal atoms. Also called glycaric acids. Names are formed by changing the '-ose' ending of the aldose names to '-aric acid'. See *carbohydrates*

aldehydes Compounds RCHO. Named using the suffixes '-al' (denoting =O) or '-carboxaldehyde' (denoting –CHO) or using the substituent prefixes 'formyl' (denoting –CHO) or 'oxo' (denoting =O). The suffix '-aldehyde' can replace the '-ic acid' or '–oic acid' or a trivially named acid; thus, benzaldehyde is PhCHO

-aldehydic acid Denotes that one COOH group of a trivially named dicarboxylic acid has been replaced by a CHO group. Thus, malonaldehydic acid is $OHCCH_2COOH$

aldehydo- Occasionally used in place of a locant in order to denote unambiguously the position of a functional derivative. For example, α-oxobenzeneacetaldehyde *aldehydo*-hydrazone is $PhC(O)CH=NHNH_2$

aldimines Imines derived from aldehydes. $R^1CH=NR^2$

alditols Polyhydric alcohols derived from aldoses by reduction of the carbonyl group. Names are formed by changing the '-ose' ending of the aldose names to '-itol'. See *carbohydrates*

aldonic acids Monocarboxylic acids formed by oxidation of the aldehyde functions of aldoses. Names are formed by changing the '-ose' ending of the aldose names to '-onic acid'. See *carbohydrates*

aldoses Monosaccharides containing an aldehyde group. Aldofuranoses, aldopyranoses and aldoseptanoses are the cyclic forms with ring sizes of five, six and seven, respectively. See *carbohydrates*

aldoximes Oximes derived from aldehydes. RCH=NOH

alkaloids The term 'alkaloid' originally signified nitrogenous bases found in plants. It is now applied to the majority of nitrogen compounds occurring in the plant or animal kingdoms. Abbreviated entries for the most widespread and important alkaloids such as berberine, coniine and strychnine are given in DOC 6. For a comprehensive treatment of all known alkaloids, see the *Dictionary of Natural Products*

alkanes General name for saturated acyclic hydrocarbons (branched or unbranched)

alkenes General name for acyclic hydrocarbons having one or more double bonds

alkoxides General term for metal salts of alcohols

alkoxy (alkyloxy) General term for the radical RO– (R = alkyl)

alkyl General term for a univalent radical derived from an alkane by removal of one hydrogen

alkylidene General term for a divalent radical derived from an alkane by removal of two hydrogens from the same carbon atom

alkylidyne General term for a trivalent radical derived from an alkane by removal of three hydrogens from the same carbon atom

alkynes General term for acyclic hydrocarbons having one or more triple bonds

allenes General term for substances containing the C=C=C unit. The lowest member, propadiene ($H_2C{=}C{=}CH_2$), is known as 'allene'

allo- (Greek 'other') A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*. Also as a general prefix to denote close relationship, e.g. alloaromadendrene or the more stable of a pair of geometric isomers, e.g. allomaleic acid (obsol.) = fumaric acid

allyl 2-propenyl $H_2C{=}CCH_2$

β-allyl (1-methylethenyl) $H_2C{=}C(CH_3)–$

allylidene 2-propenylidene $H_2C{=}CHCH{=}$

altro- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

-amic acid Denotes that one COOH group of a trivially named dicarboxylic acid has been replaced by a $CONH_2$ group. Thus, succinamic acid is $H_2NCOCH_2CH_2COOH$

amides Compounds derived from acids by replacement of a hydroxy group by NH_2. In names, the suffix '-amide' replaces the '-ic acid' or '-oic acid' of the acid name. Thus butanamide is $H_3CCH_2CH_2CONH_2$, benzamide is $PhCONH_2$, and methanesulfonamide is $MeSO_2NH_2$. In DOC 6, most amides appear as derivatives of the parent acids. The term 'amide' is also used to denote a metal derivative of an amine; thus, lithium diethylamide is Et_2NLi

amidines Compounds of the type $RC(=NH)NH_2$. The ending '-amidine' can replace the '-ic acid' or '-oic acid' of the name of the acid RCOOH. Thus, acetamidine is $H_3CC(=NH)NH_2$

amidino (aminoiminomethyl) $H_2NC(=NH)–$

amido Denotes a radical formed by loss of a hydrogen from an amide group. Thus, acetamido is $H_3CCONH–$

amidoximes (amide oximes) Oximes of carboxamides or amides derived from hydroximic acids, i.e. $RC(NH_2){=}NOH$ or $RC(=NH)NHOH$

amidrazones (amide hydrazones) Hydrazones of carboxamides or hydrazides of hydroximic acids, i.e. $RC(NH_2){=}NNH_2$ or $RC(=NH)NHNH_2$

aminals *gem*-Diamines, i.e. $R_2C(NR_2)_2$ (R is the same or different)

amine oxides Compounds $R_3N(O)$ (R is the same or different). Thus, trimethylamine oxide is Me_3NO

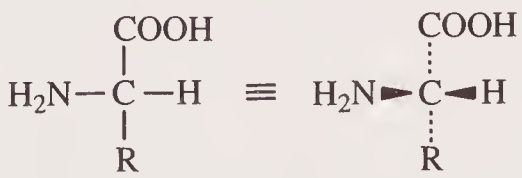
amines Compounds of the type R^1NH_2 (primary amines), R^1R^2NH (secondary amines) and $R^1R^2R^3N$ (tertiary amines). As a suffix, '-amine' may be attached either to the name of a radical or to the name of a parent compound. Thus, butylamine and 1-butanamine are both H_3CCH_2-$CH_2CH_2NH_2$. The compound H_3CCH_2CH-$(NH_2)CH_3$ is either 1-methylpropylamine or 2-butanamine (the latter is preferred in CAS). Secondary or tertiary amines having identical radicals attached to the nitrogen atom can be given names such as diethylamine (Et_2NH) and triethylamine (Et_3N)

-aminium Suffix denoting $–N^+H_3$. Thus, ethanaminium is EtN^+H_3

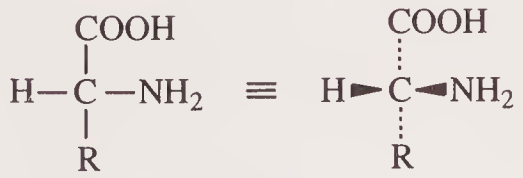
amino $H_2N–$

amino acids An important class of biochemicals that are the basis of peptide and protein structures. For full details of the nomenclature and symbolism of amino acids, see *Pure Appl. Chem.*, 1984, **56**, 595

In α-amino acids, the L-compounds are those in which the NH_2 group is on the left-hand side of the Fischer projection in which the COOH group appears at the top.



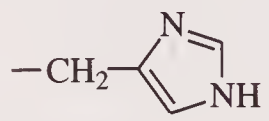
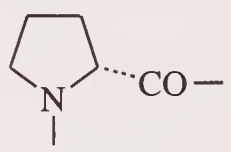
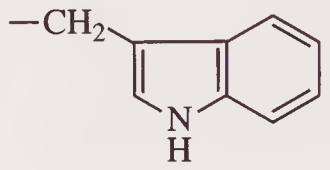
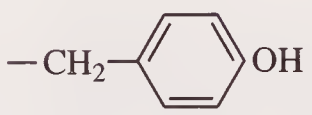
L-form



D-form

Table 8.1 lists the α-amino acids that are commonly found in peptides and proteins. The three-letter and one-letter abbreviations are those

Table 8.1 The α-amino acids commonly found in peptides and proteins

Name	Abbrevs.		R group (side-chain)	Mol. formula
alanine	Ala	A	$-CH_3$	C_3H_7NO2
arginine	Arg	R	$-(CH_2)_3NHC(=NH)NH_2$	$C_6H_{14}N_4O_2$
asparagine	Asn	N	$-CH_2CONH_2$	$C_4H_8N_2O_3$
aspartic acid	Asp	D	$-CH_2COOH$	$C_4H_7NO_4$
cysteine	Cys	C	$-CH_2SH$	$C_3H_7NO_2S$
glutamic acid	Glu	E	$-CH_2CH_2COOH$	$C_5H_9NO_4$
glutamine	Gln	Q	$-CH_2CH_2CONH_2$	$C_5H_{10}N_2O_3$
glycine	Gly	G	$-H$	$C_2H_5NO_2$
histidine	His	H		$C_6H_9N_3O_2$
isoleucine	Ile	I	$-CH(CH_3)CH_2CH_3$	$C_6H_{13}NO_2$
leucine	Leu	L	$-CH_2CH(CH_3)_2$	$C_6H_{13}NO_2$
lysine	Lys	K	$-(CH_2)_4NH_2$	$C_6H_{14}N_2O_2$
methionine	Met	M	$-CH_2CH_2SCH_3$	$C_5H_{11}NO_2S$
phenylalanine	Phe	F	$-CH_2Ph$	$C_9H_{11}NO_2$
proline (an imino acid)	Pro	P		$C_5H_9NO_2$
serine	Ser	S	$-CH_2OH$	$C_3H_7NO_3$
threonine	Thr	T	$-CH(OH)CH_3$	$C_4H_9NO_3$
tryptophan	Trp	W		$C_{11}H_{12}N_2O_2$
tyrosine	Tyr	Y		$C_9H_{11}NO_3$
valine	Val	V	$-CH(CH_3)_2$	$C_5H_{11}NO_2$

which are used in representing peptides and proteins. For all the amino acids in the table, except for cysteine, the L-form has the (*S*)-configuration. For cysteine, the L-form has the (*R*)-configuration, because the $-CH_2SH$ group has higher priority than –COOH according to the Sequence Rule. All the amino acids in this table have extensive DOC 6 entries. A large number of other 'secondary' amino acids also appear in plants and bacterial products. Some of these have DOC 6 entries, but for a full treatment see the *Dictionary of Natural Products.*

Other one-letter abbreviations are as follows:

B asparagine or aspartic acid

X unspecified amino acid

Z glutamine or glutamic acid

Other abbreviations that may be encountered in the literature include those listed in Table 8.2.

ammonio $H_3{}^+N-$

-amoyl Denotes a radical derived by loss of a hydroxy group from an amic acid. Thus, succinamoyl is $H_2NCOCH_2CH_2CO-$

amphi (Greek 'around') For example, *amphi*-naphthoquinone) (obsol.) = 2,6-naphthoquinone

amyl pentyl $H_3C(CH_2)_4-$

***tert*-amyl** (1,1-dimethylpropyl) $H_3CCH_2C(CH_3)_2-$

-ane With a numerical prefix, '-ane' denotes a

Table 8.2 Other 'amino acid-related' abbreviations that may be found in the literature

βAad	3-aminoadipic acid
Aad	2-aminoadipic acid
A2bu	2,4-diaminobutyric acid
Abu	2-aminobutanoic acid
εAhx	6–aminohexanoic acid
Ahx	2-aminohexanoic acid (norleucine)
2-MeAla	2-methylalanine
βAla	β-alanine
Ape	2-aminopentanoic acid (norvaline)
A2pm	2,6-diaminopimelic acid
Apm	2-aminopimelic acid
A2pr	2,3-diaminopropionic acid
$Asp(NH_2)$	asparagine
Asx	asparagine or aspartic acid
Avl	2-aminopentanoic acid (norvaline)
Cit	citrulline
Cya	cysteic acid
Dab	2,4-diaminobutyric acid
Dpm	2,6-diaminopimelic acid
Dpr	2,3-diaminopropionic acid
Gla	4-carboxyglutamic acid
Glp	5-oxoproline (pyroglutamic acid)
pGlu	5-oxoproline (pyroglutamic acid)
<Glu	5-oxoproline (pyroglutamic acid)
$Glu(NH_2)$	glutamine
Glx	glutamine or glutamic acid
Hcy	homocysteine
Hse	homoserine
Hsl	homoserine lactone
Hyl	5-hydroxylysine
5Hyl	5-hydroxylysine
Hyp	4-hydroxyproline
4Hyp	4-hydroxyproline
aIle	alloisoleucine
alloIle	alloisoleucine
Iva	isovaline
Met(O)	methionine *S*-oxide
MetO	methionine *S*-oxide
$MetO_2$	methionine *S,S*-dioxide
Mur	muramic acid
Neu	neuraminic acid
Neu5Ac	*N*-acetylneuraminic acid
Nle	norleucine
Nva	norvaline
Orn	ornithine
5-oxo-Pro	5-oxoproline (pyroglutamic acid)
Sar	sarcosine
Ser(P)	phosphoserine
alloThr	allothreonine
aThr	allothreonine
Thx	thyroxine
$Tyr(I_2)$	3,5-diiodotyrosine
$Tyr(SO_3H)$	O^4-sulfotyrosine
Xaa	unspecified amino acid

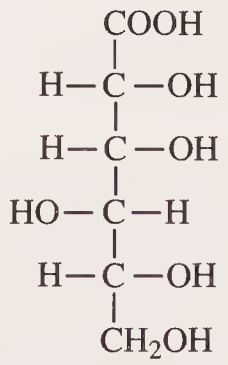
saturated hydrocarbon, e.g. pentane, hexane. Also, a Hantzsch–Widman stem for a six-membered saturated ring containing no nitrogen (e.g. dioxane)

ang- Prefix for angular, i.e. referring to an angular isomer (obsol.)

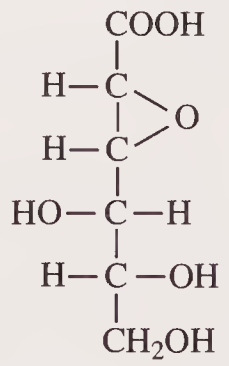
angeloyl (*Z*)-(2-methyl-1-oxo-2-butenyl) $(Z)\text{-}H_3CCH{=}C(CH_3)CO–$ The (*E*)-form is 'tigloyl'

anhydrides Compounds derived by the elimination of the elements of water from two acid molecules. Thus, acetic anhydride is $(H_3CCO)_2O$ and acetic benzoic anhydride is $H_3CCOOCOPh$. Cyclic anhydrides, e.g. succinic anhydride, are formed by the elimination of the elements of water from the OH groups of a dibasic acid

anhydro A subtractive prefix denoting the loss of the elements of water within one molecule



D-gulonic acid



2,3-anhydro-D-gulonic acid

anhydrosulfide An analogue of an anhydride in which the oxygen atom connecting the two acyl residues has been replaced by a sulfur atom. Anhydroselemides are the Se analogues

-anilic acid Denotes that one COOH group of a trivially named dicarboxylic acid has been replaced by a CONHPh group. Thus, succinanilic acid is $PhNHCOCH_2CH_2COOH$

anilides *N*-phenyl amides RCONHP They may be named by replacing the '-ic acid' or '-oic acid' in the name of the acid RCOOH by '-anilide'. Thus, acetanilide is $H_3CCONHPh$. Primed locants are used for the phenyl ring

anilino (phenylamino) PhNH–

anils Another term for azomethine compounds or Schiff bases. Sometimes restricted to *N*-phenylimines $PhN{=}CR_2$

anisoyl (methoxybenzoyl) Thus, *O*-anisoyl is $2\text{-}MeOC_6H_4CO–$

annulenes Monocyclic conjugated hydrocarbons with the general formula $(CH)_n$. Thus [8]annulene is cyclooctatetraene

anomers Two stereochemical configurations, known as anomers, may result from the formation of cyclic forms of monosaccharides. They are distinguished by the anomeric prefixes α- and β-. See *carbohydrates*

ansa compounds (Greek 'handle') Compounds containing a ring system bridged by an aliphatic chain. The simplest type consists of a benzene ring with the *para* positions bridged by a methylene chain 10–12 atoms long

anthocyanins Flavonoid pigments of glycosidic nature. On hydrolysis they give anthocyanidins, which are oxygenated, derivatives of flavylium salts. For further information, see the *Dictionary of Natural Products*

anthra The ring fusion prefix derived from anthracene

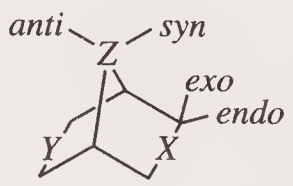
anthraniloyl or **anthranoyl** (2-aminobenzoyl) $2\text{-}H_2NC_6H_4CO–$

anthroyl (anthracenylcarbonyl) $(C_{14}H_9)CO–$

anthryl anthracenyl $(C_{14}H_9)–$

anthrylene anthracenediyl $–(C_{14}H_8)–$

anti (Greek 'opposite') Stereochemical descriptor used for bridged bicyclic compounds. In a bicyclo[*X.Y.Z*] compound ($X \geq Y > Z$), *anti*- denotes that a substituent on the *Z* bridge points away from the *X* bridge.



anti- is equivalent to *trans*- or (*E*)- when used to indicate the stereochemistry of oximes and similar C=N compounds. (obsol. : use *E* or *Z*)

apo (Greek 'from') In general means 'derived from', e.g. apomorphine. Oxidative degradation products of carotenes can be named as 'apo' carotenoids. The prefix 'apo' preceded by a locant is used to indicate that all of the molecule beyond the carbon atom corresponding to that locant has been replaced by a hydrogen atom. The prefix 'diapo' is used to indicate removal of fragments from both ends of the molecule

ar- Abbreviation for '*aromatic*, used as a locant to indicate an attachment at an unspecified position on an aromatic ring. Thus, in *ar*-methylaniline the methyl group is attached to the aromatic ring and not to the amine N atom

Ar Often used in structural formulae to denote an unspecified aryl group

appendage A structural subunit consisting of one or more carbon atoms and their substituents, which is bonded to a ring or functional group

arabino A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

aralkyl A general name for a radical comprising an aryl group attached to an alkyl radical, e.g. $PhCH_2CH_2–$

arenes A general name for monocyclic and polycyclic aromatic hydrocarbons

arginyl $H_2NC(=NH)NH(CH_2)_3CH(NH_2)CO–$ The acyl radical from arginine used in naming peptides

-aric acid See *aldaric acids*

arsa Replacement prefix denoting arsenic. See the *Dictionary of Organometallic Compounds* for full coverage of organoarsenic compounds

aryl General term for a monovalent radical derived by loss of hydrogen from an aromatic hydrocarbon

arylene General term for a divalent radical derived by loss of hydrogens from two different atoms of an aromatic hydrocarbon

as- Abbreviation for asymmetric, as in *as*-triazine (1,2,4-triazine). Sometimes used to indicate 1,2,4-substitution on an aryl ring, e.g. *as*-trichlorobenzene is $1,2,4\text{-}Cl_3C_6H_3$

asaryl 2,4,5-trimethoxyphenyl

asparaginyl $H_2NCOCH_2CH(NH_2)CO–$ The acyl radical from asparagine, used in naming peptides

aspartoyl The diradical $–COCH_2CH(NH_2)CO–$

aspartyl May refer either to aspartoyl or to unspecified aspartyl

α-aspartyl The acyl radical $HO_2CCH_2CH(NH_2)CO–$, used in naming peptides

β-aspartyl The acyl radical $HO_2CCH(NH_2)CH_2CO–$, used in naming peptides

assembly nomenclature See *ring assemblies* and *multiplicative nomenclature*

aza Replacement prefix denoting a nitrogen atom

-azane With a numerical prefix, '-azane' denotes a chain of nitrogen atoms. Thus, triazane is H_2NNHNH_2, tetrazane is $H_2NNHNHNH_2$, etc.

azelaoyl (1,9-dioxo-1,9-nonanediyl) $–CO(CH_2)CO–$

-azene With a numerical prefix, '-azene' denotes a chain of nitrogen atoms containing one double bond. Thus, triazene is $N_2NN{=}NH$, 2-tetrazene is $H_2NN{=}NNH_2$, etc.

azi –N=N– Usually used when both free valencies are attached to the same atom

azides Compounds containing the group $–N_3$. Thus, phenyl azide is PhN_3, acetyl azide is AcN_3

azido $N_3–$

azimino –N=NNH– Used as a bridge name in naming bridged fused ring systems

azines Compounds containing the azino group. They may be named by adding the word 'azine' after the name of the corresponding aldehyde or ketone. Thus, acetone azine is $(H_3C)_2C{=}N–N{=}C(CH_3)_2$. 'Azines' is sometimes used as a general term to refer to six-membered heterocycles containing nitrogen in the ring

azino =N–N= (a multiplying radical)

azo –N=N– (a multiplying radical)

azo compounds Compounds containing the azo group. Thus, azobenzene is PhN=NPh and naphthalene-2-azobenzene is $2\text{-}C_{10}N_7N{=}NPh$. In CAS they are now named as substituted diazenes, e.g. 1-(2-naphthalenyl)-2-phenyldiazene

azoles 'Azoles' is sometimes used as a general term to refer to five-membered heterocycles containing nitrogen in the ring

azomethines Compounds with the formula $R_2C{=}NR^1$. When the N atom is substituted ($R^1 \neq H$), they are known as Schiff bases. When used as the name of a specific compound, 'azomethine' is methanimine, $H_2C{=}NH$

azonia Replacement prefix denoting a positively charged nitrogen atom

azonic acids Compounds with structure $R_2N(O)OH$

azoxy –N(O)=N– (a multiplying radical)

azoxy compounds Compounds containing the azoxy group. Thus, azoxybenzene is PhN(O)=NPh. To express the position of the azoxy oxygen atom of an unsymmetrical azoxy compound, a prefix *NNO*- or *ONN*- is used. Thus, 2-naphthyl-*NNO*-azoxybenzene is $2\text{-}C_{10}H_7N{=}N(O)Ph$ and 2-naphthyl-*ONN*-azoxybenzene is $2\text{-}C_{10}H_7N(O){=}NPh$. In CAS they are now named as diazene *N*-oxides

benzal (phenylmethylene) PhCH=

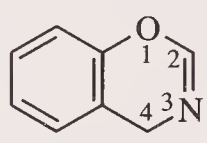
benzamido (benzoylamino) PhCONH–

benzeno $–(C_6H_4)–$ Bridge name used in naming bridged fused ring systems

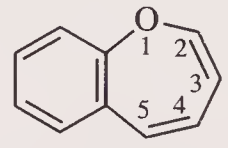
benzhydryl (diphenylmethyl) $Ph_2CH–$

benzhydrylidene (diphenylmethyl) $Ph_2C{=}$

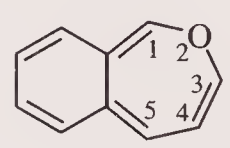
benzo The ring fusion prefix from benzene. It is used in the normal manner when naming fused systems such as benz[*a*]anthracene and benzo[*b*]thiophene. However, bicyclic hetero ring systems consisting of a benzene ring fused to a monocyclic hetero ring named by the Hantzsch–Widman system (*q.v.*) receive a slightly different treatment. 'Benzo' or 'benz' is placed directly in front of the Hantzsch–Widman name of the monocyclic hetero ring and indicated hydrogen and locants describing the position of the heteroatoms are cited, when necessary, in front of the resulting name



4*H*-1,3-benzoxazine



1-benzoxepin



1-benzoxepin

benzoyl PhCO– Often abbreviated to Bz in structural and line formulae

benzyl (phenylmethyl) $PhCH_2–$

benzylidene (phenylmethylene) PhCH=

benzylidyne (phenylmethylidyne) PhC≡

betaine Trivial name for zwitterionic compounds characterised by $Me_3N^+CH_2COO^-$. 'Betaines' is also used as a class name for similar compounds containing a cationic centre and an anionic centre; they are also called 'inner salts' and 'zwitterionic compounds'. Named as 'hydroxide, inner salts' in CA

bi Used in names of ring assemblies (see *ring assemblies*) and in von Baeyer names of bridged bicyclic systems (see *von Baeyer nomenclature*). Also used to denote the doubling of an alicyclic radical or molecule as in biacetyl ($H_3CCOCOCH_3$) and bicarbamic acid (HOOCNHNHCOOH)

bicyclo For an explanation of names like bicyclo-[2.2.1]heptane, see *von Baeyer nomenclature*. Names like bicyclohexyl denote ring assemblies (see *ring assemblies*)

biimino –NH–NH– Used in naming bridged fused ring systems

bile pigments A class of compounds possessing a linear tetrapyrrolic structure, the four pyrrole rings of which are connected by single carbon atoms.

Further information can be found in the *Dictionary of Natural Products*

bis Numerical prefix denoting 'two'. Used instead of 'di' with complex terms and to avoid ambiguity

bisnor See *nor*

bora Replacement prefix denoting boron

borane BH_3

borinic acid $H_2B(OH)$

bornyl A contracted form of bornanyl, the radical derived from bornane

boronic acid $HB(OH_{2)}$

borono $(HO)_2B–$

boryl $H_2B–$

borylene HB=

borylidyne B≡

Boughton system A system for naming isotopically labelled compounds. See *labelled compounds*

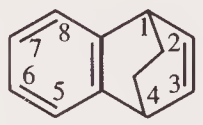
bridged ring systems Many bridged ring systems are named by the von Baeyer system (see *von Baeyer nomenclature*); an example is bicyclo-[2.2.1]heptane.

Fused ring systems that have other bridges are usually named by prefixing the name of the bridge to the name of the fused ring system. The names of hydrocarbon bridges are derived from the names of the parent hydrocarbons by replacing the final '-ane', '-ene', etc. by 'ano', '-eno', etc. Thus, $–CH_2–$ is methano and –CH=CH– is etheno.

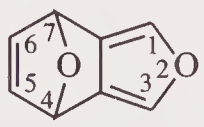
Names for bridges containing heteroatoms include:

–O–	epoxy
–S–	epithio
–NH–	imino
–N=N–	azo
–O–O–	epidioxy
–S–S–	epidithio
–N=	nitrilo
$–OCH_2–$	(epoxymethano)

Some examples are the following:



1,4-dihydro-1,4-ethanonaphthalene



4,7-dihydro-4,7-epoxyisobenzofuran

bromo Br–

bromonio $H^+Br–$

bromonium H_2Br^+

brosyl *p*-bromobenzenesulfonyl

Bunte salts Salts of *S*-alkyl thiosulfates with structure $RSS(O)_2O^-M^+$

butiodide, butobromide, butochloride Indicates a base quaternised with butyl iodide, butyl bromide or butyl bromide

butoxide or **n-butoxide** The anion BuO^-. Thus, sodium butoxide is BuONa. Similarly, *sec*-butoxide is Bu^sO^- and *tert*-butoxide is Bu^tO^-

butoxy or **n-butoxy** $H_3CCH_2CH_2CH_2O–$

***sec*-butoxy** (1-methylpropoxy) $H_3CCH_2CH(CH_3)O–$

***tert*-butoxy** (1,1-dimethylethoxy) $(H_3C)_3CO–$

butyl or **n-butyl** $H_3CCH_2CH_2CH_2–$ Often abbreviated to Bu (or *n*-Bu or Bu^n) in structural formulae

***sec*-butyl** (1-methylpropyl) $H_3CCH_2CH(CH_3)–$ Often abbreviated to Bu^s or *s*-Bu in structural formulae

***tert*-butyl** (1,1-dimethylethyl) $(H_3C)_3C–$ Often abbreviated to Bu^t or *t*-Bu in structural formula.

butylidene $H_3CCH_2CH_2CH=$

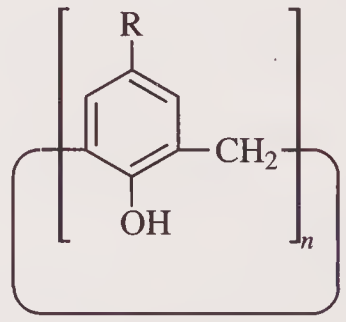
***sec*-butylidene** (1-methylpropylidene) $H_3CCH_2C(CH_3)=$

butylidyne $H_3CCH_2CH_2C≡$

butyryl (1-oxobutyl) $H_3CCH_2CH_2CO–$

***c*-** Abbreviation for *cis*-

calixarenes Cyclic oligomers formed from *para*-substituted phenols and formaldehyde



calixarenes

Shinkai, S., *Tetrahedron*, 1993, **49**, 8933

Gutsche, C. D., *Calixarenes*, Monographs in Supramolecular Chemistry, ed. J. F. Stoddart, Royal Society of Chemistry, London, 1989

Vicens, J., *Calixarenes, a Versatile Class of Macrocyclic Compounds*, Kluwer, Dordrecht, 1991

caprinoyl (1-oxodecyl) $H_3C(CH_2)_8CO–$

caproyl (1-oxohexyl) $H_3C(CH_2)_4CO–$

capryl (1-oxodecyl) $H_3C(CH_2)_8CO–$ 'Capryl' has also been used to mean octyl, $H_3C(CH_2)_7–$

capryloyl or **caprylyl** (1-oxooctyl) $H_3C(CH_2)_6CO–$

carba Occasionally used as a replacement prefix indicating that a carbon atom has replaced a heteroatom. For an example see *carbapenam*

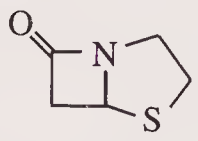
-carbaldehyde Contracted form of '-carboxaldehyde'

carbamido [(aminocarbonyl)amino] $H_2NCONH–$

carbamoyl or **carbamyl** (aminocarbonyl) $H_2NCO–$

carbaniloyl [(phenylamino)carbonyl] $PhNHCO–$

carbapenams Penams in which the sulfur atom has been replaced by a carbon



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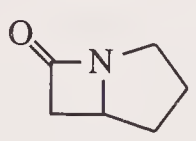


carbapenam

carbazoyl (hydrazinocarbonyl) $H_2NNHCO–$

carbenes Used as a general name for a type of neutral species in which the carbon atom is covalently bonded to two groups and also bears two non-bonding electrons, i.e. derivatives of methylene, $:CH_2$

carbethoxy (ethoxycarbonyl) EtOOC–

carbinol Once used as the name for the parent H_3COH in naming substituted alcohols. Thus, diphenylcarbinol is Ph_2CHOH and triethylcarbinol is $(H_3CCH_2)_3COH$

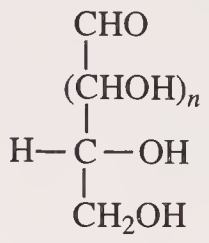
carbobenzoxy [(phenylmethoxy)carbonyl] $PhCH_2OOC–$

-carbodithioic acid Suffix denoting –C(S)SH

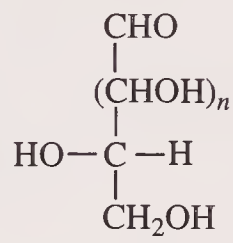
carbohydrates Comprise a family of polyhydroxy aldehydes, ketones and acids, together with linear and cyclic polyols. Entries for all of the fundamental carbohydrates (mono- and disaccharides)and many of their derivatives are given in DOC 6. For a comprehensive treatment of naturally occurring carbohydrates, see the *Dictionary of Natural Products*. Some aspects of the naming of carbohydrates are given below. Further details can be found in *Biochemistry*, 1971, **10**, 3983, 4995

Numbering of monosaccharides. Open-chain carbohydrates containing an aldehyde function are numbered so that the aldehyde function is at carbon number 1. When an aldehyde function is not present, the highest-ranking function is given the lowest possible locant.

In a *Fischer projection* (*q.v.*) of an open-chain carbohydrate, the chain is written vertically with carbon number 1 at the top. The hydroxyl group on the highest-numbered asymmetric carbon atom is depicted on the right in monosaccharides of the D-series and on the left in the L-series.



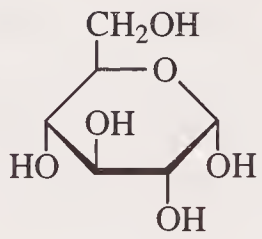
D-form



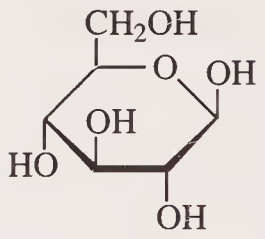
L-form

When a monosaccharide exists in the heterocyclic intramolecular hemiacetal form, the size of the ring is indicated by the suffixes '-furanose', '-pyranose' and '-septanose' for five-, six- and seven-membered rings, respectively.

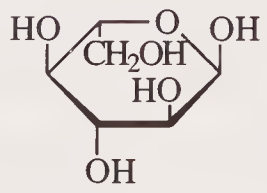
Two configurations, known as anomers, may result from the formation of the ring. These are distinguished by the anomeric prefixes 'α-' and 'β-', which relate the configuration of the anomeric carbon atom to the configuration at a reference chiral carbon atom (normally the highest-numbered chiral carbon atom). The *Haworth representation* (*q.v.*) is often used for the cyclic forms of monosaccharides. For example, consider the glucopyranoses:



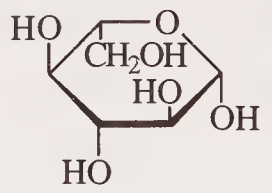
α-D-



β-D-



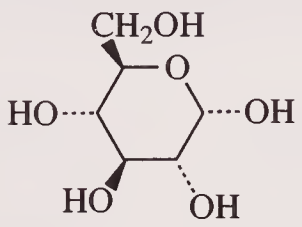
α-L-



β-L-

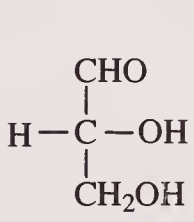
- In the D-series, the CH_2OH is projected above the ring.
- In the L-series, the CH_2OH is projected below the ring.
- In the α-series, the anomeric OH (at position 1) is on the opposite side of the ring to the CH_2OH group.
- In the β-series, the anomeric OH (at position 1) is on the same side of the ring as the CH_2OH group.

These can also be represented as planar hexagon formulae:

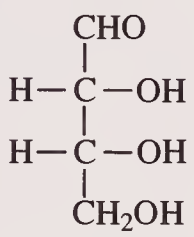


α-D-glucopyranose

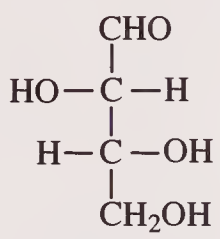
Trivia names for the adoses and their formulae are:



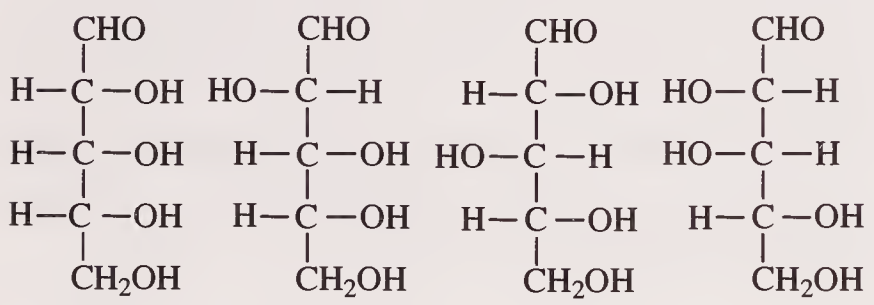
D-glycerose



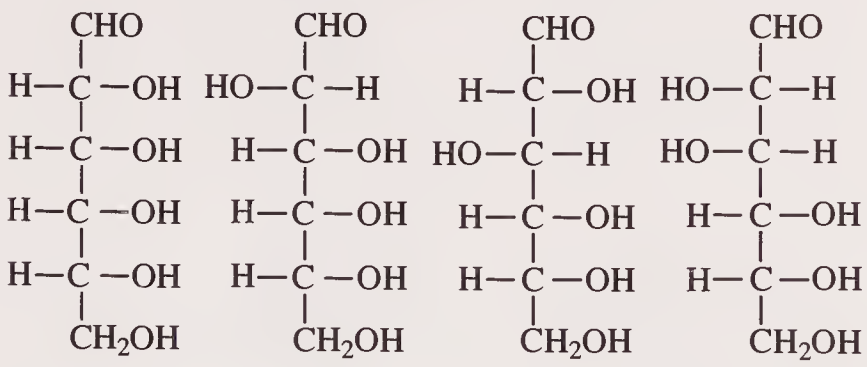
D-erythrose



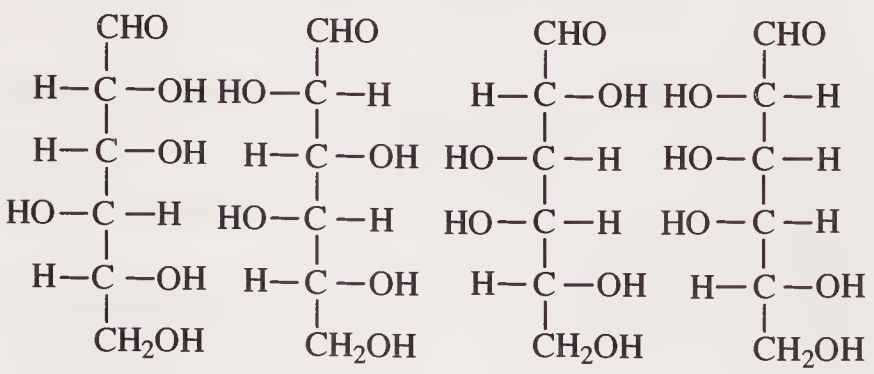
D-threose



D-ribose D-arabinose D-xylose D-lyxose

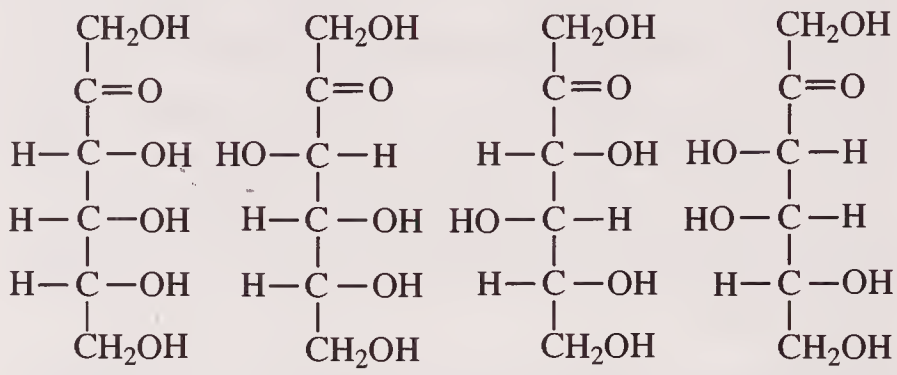


D-allose D-altrose D-glucose D-mannose



D-gulose D-idose D-galactose D-talose

Trivial names for the 2-hexuloses and their formulae are:



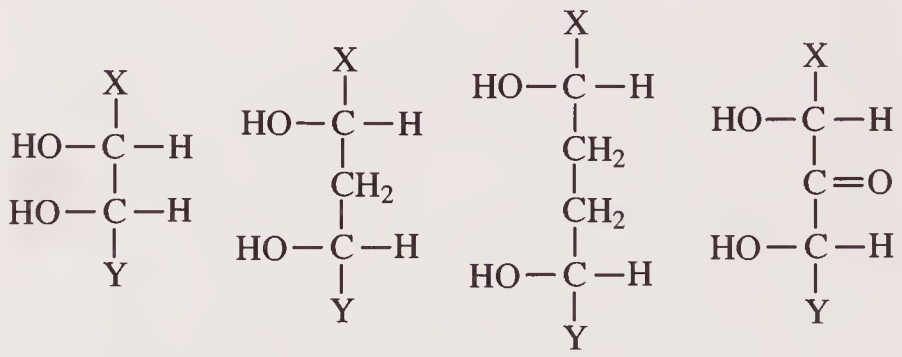
D-psicose D-fructose D-sorbose D-tagatose

In *systematic carbohydrate nomenclature*, the configuration of a group of consecutive, but not necessarily contiguous, asymmetric carbon atoms (such as >CHOH) containing one to four asymmetric centres is designated by one of the following configurational prefixes.

No. of carbon atoms	Prefixes
1	*glycero-*
2	*erythro-*, *threo-*
3	*arabino-*, *lyxo-*, *ribo-*, *xylo-*
4	*allo-*, *altro-*, *galacto-*, *gluco-*, *gulo-*, *ido-*, *manno-*, *talo-*

Each prefix is preceded by the D- or L- depending on the configuration of the highest-numbered asymmetric carbon atom in the Fischer projection of the prefix.

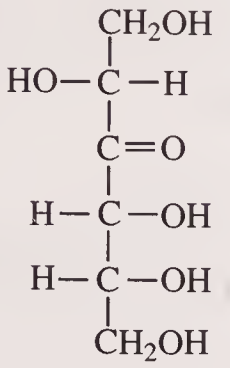
The consecutive asymmetric carbon atoms do not need to be contiguous. Thus the following four arrangements are all L-*erythro*- ('X' is attached to the lowest-numbered carbon atom).



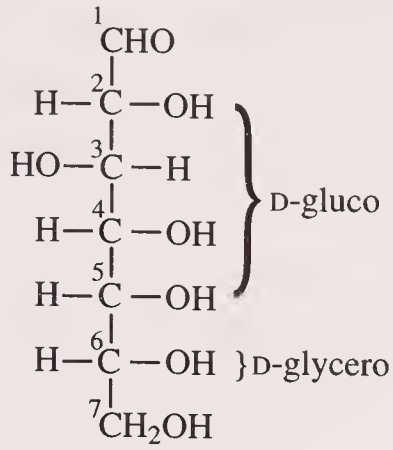
L-*erythro*-

Sugars having more than six carbon atoms are named using two prefixes, one defining the configuration at C(2)–C(5) as in a hexose, and the other, which appears first in the name, defining the configuration at the remaining chiral centres.

Examples of the use of configurational prefixes are:



D-*arabino*-3-hexulose



D-*glycero*-D-*gluco*-heptose

Suffixes used in carbohydrate nomenclature are given in Table 8.3. Examples of endings for cyclic forms are:

-ose	-opyranose
-ulose	-ulopyranose
-osulose	-opyranosulose or -osulopyranose
-odialdose	-odialdopyranose

The suffixes for the acids can be modified to indicate the corresponding amides, nitriles, acid halides, etc. e.g. '-uronamide', '-ononitrile', '-ulosonyl chloride'.

Abbreviations for use in representing oligosaccharides are shown in Table 8.4. See *Pure Appl. Chem.*, 1982, **54**, 1517

Examples are:

Ara*f*	arabinofuranose
Glc*p*	glucopyranose
Gal*p*A	galactopyranuronic acid
D-Glc*p*N	2-amino-2-deoxy-D-glucopyranose
3,6-AnGal	3,6-anhydrogalactose

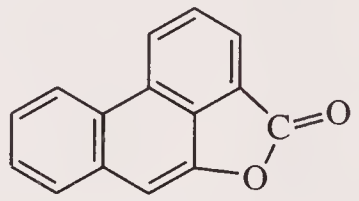
carbogen Any carbon-containing molecule, source of carbon fragments in synthesis

-carbohydrazonic acid Suffix denoting $-C(OH)=NNH_2$

-carbohydroxamic acid Suffix denoting $-C(=NOH)OH$

-carbohydroximic acid Suffix denoting $-C(O)NHOH$

-carbolactone Suffix denoting the presence of a lactone ring fused to a ring system



1,10-phenanthrenecarbolactone

carbomethoxy (methoxycarbonyl) MeOOC–

carbonimidoyl $-C(=NH)-$ (multiplying radical)

-carbonitrile Suffix denoting $-C\equiv N$

–carbonitrolic acid Suffix denoting $-C(=NOH)NO_2$

-carbonitrosolic acid Suffix denoting $-C(=NOH)NO$

carbonium compounds Electron-deficient, positively charged, tricoordinate carbon atoms. For example, H_3C^+ is methylium, $C_6H_5^+$ is phenylium

carbonothioyl $-C(S)-$ (multiplying radical)

carbonyl $-C(O)-$

-carbonyl Denotes a radical formed from a carboxylic acid and used in naming acid halides, etc. Thus, cyclohexanecarbonyl is $C_6H_{11}CO-$ and cyclohexanecarbonyl chloride is $C_6H_{11}COCl$

Table 8.3 Suffixes used in carbohydrate nomenclature

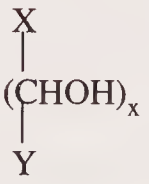
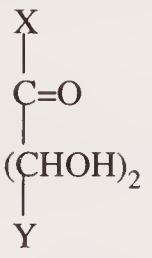
-ose	aldose	X = CHO, Y = CH_2OH	
-odialdose	dialdose	X = Y = CHO	
-onic acid	aldonic acid	X = COOH, Y = CH_2OH	
-uronic acid	uronic acid	X = CHO, Y = COOH	
-aric acid	aldaric acid	X = Y = COOH	
-itol	alditol	X = Y = CH_2OH	
-ulose	ketose	X = Y = CH_2OH	 (2-hexulose series)
-osulose	ketoaldose	X = CHO, Y = CH_2OH	
-ulosonic acid	ulosonic acid	X = COOH, Y = CH_2OH	
-ulosuronic acid	ulosuronic acid	X = CHO, Y = COOH	
-ulosaric acid	ulosaric acid	X = Y = COOH	
-odiulose	diketose		

Table 8.4 Abbreviations for use in representing oligosaccharides

hexoses	All	allose
	Alt	altrose
	Gal	galactose
	Glc	glucose
	Gul	gulose
	Ido	idose
	Man	mannose
	Tal	talose
pentoses	Ara	arabinose
	Lyx	lyxose
	Rib	ribose
	Xyl	xylose
other	Rha	rhamnose
	Fuc	fucose
	Fru	fructose
suffixes	*f*	furanose
	p	pyranose
	A	uronic acid
	N	2-deoxy-2-amino sugar
prefixes	D-	configurational descriptor
	L-	configurational descriptor
	An	anhydro

carbonyl compounds Compounds containing a carbonyl group. Often restricted to aldehydes and ketones

-carbonyl halide Suffix denoting C(O)X (X = halogen). For example, '-carbonyl chloride' denotes –C(O)Cl

-carboperoxoic acid Suffix denoting –C(O)OOH

carboranes A contraction of carbaboranes. Compounds in which a boron atom in a polyboron hydride is replaced by a carbon atom

-carboselenaldehyde Suffix denoting –C(=Se)H

-carboselenoic acid Suffix denoting –C(=Se)OH or –C(=O)SeH

-carboselenothioic acid Suffix denoting –C(=Se)SH or –C(=S)SeH

-carbothioaldehyde Suffix denoting –C(=S)H

-carbothioamide Suffix denoting $-C(=S)NH_2$

-carbothioic acid Suffix denoting –C(=S)OH (-carbothioic *O*-acid) or –C(O)SH (-carbothioic *S*-acid)

-carboxaldehyde Suffix denoting –CHO

-carboxamide Suffix denoting $-CONH_2$

-carboxamidine Suffix denoting $-C(=NH)NH_2$

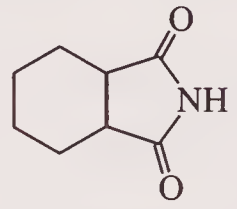
-carboxamidoxime Suffix denoting $-C(=NOH)NH_2$

-carboxamidrazone Suffix denoting $-C(=NHNH_2)NH_2$

-carboxanilide Suffix denoting –CONHPh

-carboximidamide Suffix denoting $-C(=NH)NH_2$

-carboximide or **-dicarboximide** Suffix denoting an imide of a dicarboxylic acid



1,2-cyclohexanedicarboximide

-carboximidic acid Suffix denoting –C(=NH)OH

carboxy HOOC–

-carboxylic acid Suffix denoting –COOH. Carboxylic acids are compounds RCOOH

carbylamines Isocyanides (obsol.)

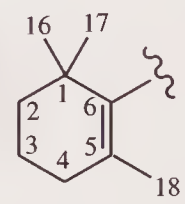
carbynes Neutral species, R–C, in which the carbon atom is covalently bonded to one group and also bears three non-bonding electrons

carceplex A complex formed by a carcerand
Cram, D. J., *et al. J. A. C. S.*, 1994, **116**, 111
Chapman, R. G., *et al.*, *J. A. C. S.*, 1994,**116**, 369

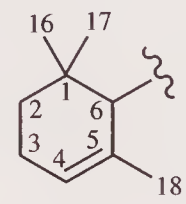
carcerand A globular molecule capable of encapsulating smaller molecules in its interior cavity

carotenoids A class of hydrocarbons consisting of eight isoprenoid units. For a comprehensive treatment of carotenoids, see the *Dictonary of Natural Products.*

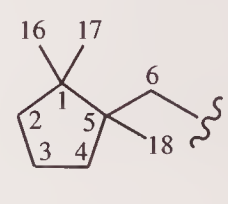
The name of a specific carotenoid hydrocarbon is constructed by adding two Greek letters as prefixes to the stem name 'carotene', these



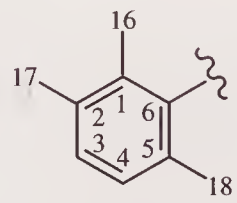
β-



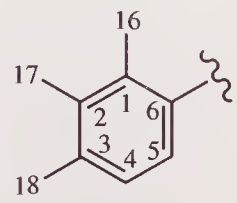
ε-



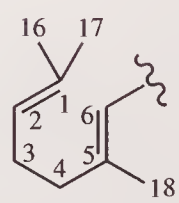
κ-



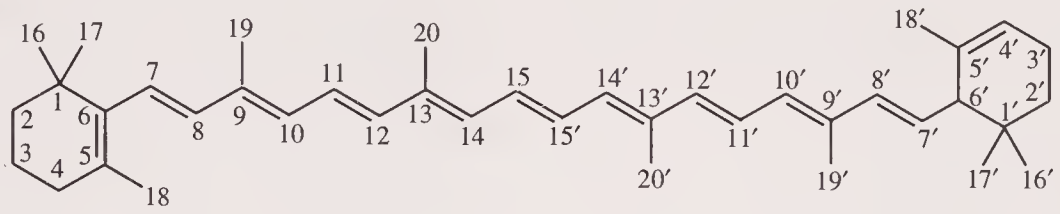
ϕ-



χ-



ψ-



β,ε-carotene

prefixes being characteristic of the two C_9 end-groups. The prefixes are: β- (beta), ε- (epsilon), κ- (kappa), φ– (phi), χ– (chi) and ψ- (psi).

For example, β,ε-carotene is as above:

catecholamines Derivatives of 4-(2-aminoethyl)-1,2-benzenediol

catenanes Compounds having two or more rings connected in the manner of the links of a chain, without a covalent bond between the rings

cathyl (ethoxycarbonyl) EtOC(O)–

cavitand A compound containing a geometrically enforced cavity large enough to accommodate simple molecules or ions

Cram, D. J., *Container Molecules and Their Guests,* Royal Society of Chemistry, London, 1994

ceramides *N*-Acylated sphingoids. See *sphingoids*

cetyl Hexadecyl $H_3C(CH_2)_{15}$–

chalcones (chalkones) Substituted derivatives of the parent compound 1,3-diphenyl-2-propen-1-one, PhCH=CHCOPh

chiral auxiliary (chiral controller) A chiral structural unit that, when attached to a molecule, enhances stereoselectivity in the formation of new stereocentre(s)

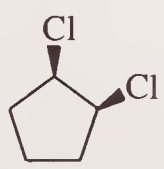
chloride 'Chloride' is used in radicofunctional names. Thus, ethyl chloride is EtCl and benzoyl chloride is PhCOCl. It can also be used in additive names; thus, ethylene dichloride is $ClCH_2CH_2Cl$

cinnamoyl (1-oxo-3-phenyl-2-propenyl) PhCH=CHCO– Usually refers to the (*E*)- form

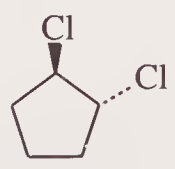
cinnamyl (3-phenyl-2-propenyl) $PhCH=CHCH_2$–

cinnamylidene (3-phenyl-2-propenylidene) PhCH=CHCH=

cis- Stereochemical descriptor denoting that two groups are on the same side of a ring or other plane

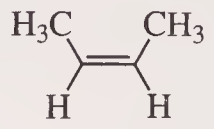


cis-1,2-dichlorocyclopentane

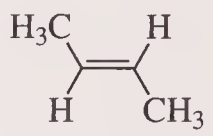


trans-

Also used to indicate the configuration of a double bond; (*Z*)- and (*E*)- are now used instead of *cis*- and *trans*-

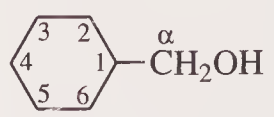


cis-2-butene
(*Z*)-2-butene

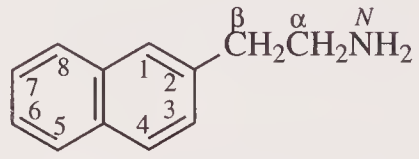


trans-2-butene
(*E*)-2-butene

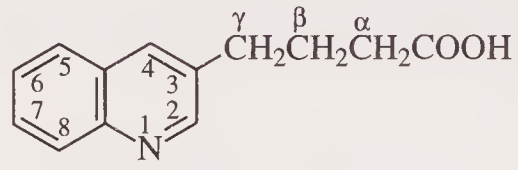
conjunctive nomenclature Much used in *Chemical Abstracts* indexes, conjunctive nomenclature may be applied when a principal group is attached to an acyclic component that is directly attached by a carbon–carbon bond to a cyclic component. A conjunctive name consists of the name of the parent ring system followed by the name of the acyclic chain plus the suffix indicating the principal group. A conjunctive name implies that hydrogen has been eliminated from each component by a process of mutual substitution. The ring system retains its normal numbering. The carbon atoms in the side-chain are indicated by Greek letters (α, β, γ, etc.) proceeding from the principal group to the cyclic component; the terminal carbon of acids, acid halides, amides, aldehydes and nitriles is omitted when allocating Greek positional letters



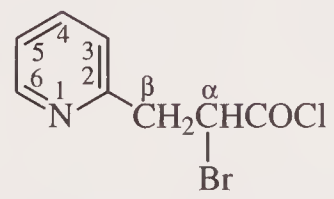
cyclohexanemethanol



2-naphthaleneethanamine

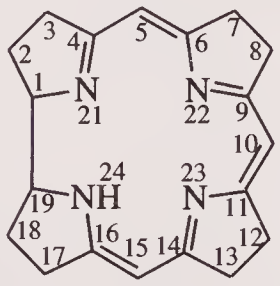


3-quinolinebutanoic acid



α-bromo-2-pyridinepropanoyl chloride

corrinoids Compounds containing the corrin nucleus.



The number 20 is *omitted* when numbering the corrin nucleus so that the numbering system will correspond to that of the porphyrin nucleus
Pure Appl. Chem., 1976, **48**, 495

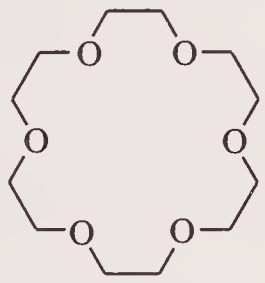
cresoxy (methylphenoxy) $H_3CC_6H_4O$–

cresyl (methylphenyl) $H_3CC_6H_3$– or (hydroxymethylphenyl) $HO(H_3C)C_6H_4$–

crotonoyl or **crotonyl** (1-oxo-2-butenyl) $H_3CCH{=}CHCO$–

crotyl 2-butenyl $H_3CCH{=}CHCH_2$–

crown ethers A class of macrocyclic ethers that form chelates with cations.



18-crown-6

The name '18-crown-6' indicates a total of 18 ring atoms including six oxygens

cumenyl Isopropylphenyl $(H_3C)_2CHC_6H_4$–

cumoyl 4-Isopropylbenzoyl 4-$(H_3C)_2CHC_6H_4CO$–

cumulenes Compounds having three or more cumulative double bonds; $R_2C{=}C{=}C{=}CR_2$

cumyl Isopropylphenyl $(H_3C)_2CHC_6H_4$

α-cumyl (1-methyl-1-phenylethyl) $PhC(CH_3)_2$–

cyanates Compounds containing the –OCN group. Thus, methyl cyanate is MeOCN

cyanato NCO–

cyanides Compounds containing the –CN group. Thus, ethyl cyanide is EtCN. The more usual name is 'nitriles'. Note that EtCN is propanenitrile

cyano NC–

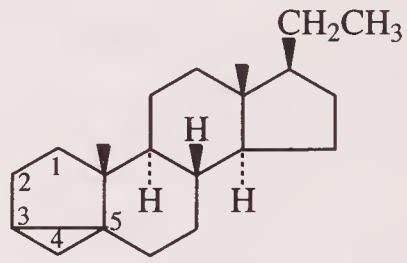
cyanohydrins Cyanoalcohols Acetone cyanohydrin is $(H_3C)_2C(OH)(CN)$; ethylene cyanohydrin is $HOCH_2CH_2CN$

cyclitols Cycloalkanes in which the hydroxyl group is attached to each ring atom. Cyclitols of the cyclohexane series constitute the inositols; see DOC 6 entries for the various members of the series

Postemak, Th., *The Cyclitols*, Holden-Day, San Francisco, 1965

Hudlicky, T. and Cebulak, M., *Cyclitols and Their Derivatives*, VCH, New York, 1993

cyclo 'Cyclo' denotes the formation of a ring by means of a direct link between two atoms with loss of one hydrogen from each; e.g. cyclohexane, cyclotrisilane. In terpene and steroid names 'cyclo-' indicates that an additional ring has been formed by means of a direct link between atoms of the fundamental skeleton



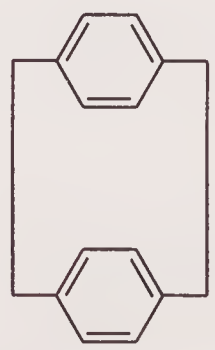
3,5-cyclopregnane

cycloalkanes General term for saturated monocyclic hydrocarbons (cyclopropane, cyclobutane, cyclopentane, etc.). Unsaturated analogues with endocyclic double and triple bonds are called cycloalkenes and cycloalkynes, respectively

cycloalkyl General term for a univalent radical formed by removal of a hydrogen from a cycloalkane. The corresponding diradical formed by removal of two hydrogens from the same atom of a cycloalkane is termed 'cycloalkylidene'

cyclodextrins Cyclic oligosaccharides consisting of α-D-(1→4)-linked D-glucose residues

cyclophanes Cyclic compounds having two or more aromatic rings with aliphatic bridging chains



2,2-[1,4]cyclophane

cysteinyl The acyl radical from cysteine $HSCH_2CH(NH_2)CO–$, used in naming peptides

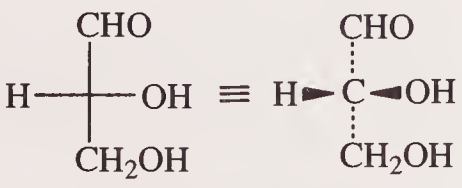
cysteyl $HO_3SCH_2CH(NH_2)CO–$

d- An abbreviation of *dextro-*. Indicates that a compound is dextrorotatory (obsol.; use should be avoided because of confusion with D-)

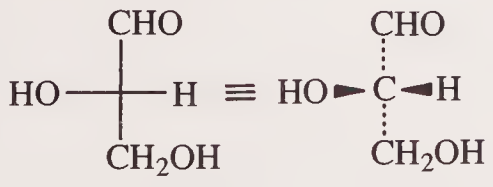
-d Denotes deuterium in the Boughton system for naming isotopically labelled compounds. See *labelled compounds*

D- D- and L- are configurational descriptors used to denote the configuration of chiral molecules, especially carbohydrates and α-amino acids. Fischer projections are used to assign the symbols D- and L-

(+)-Glyceraldehyde is defined as D-; the OH group attached to C(2) is on the right-hand side of the Fischer projection in which the CHO group appears at the top. Its enantiomer is defined as L- because the OH group is on the left-hand side. (The D- and L- symbols were originally assigned arbitrarily; in the 1950s it was found that (+)-glyceraldehyde did indeed have the absolute configuration represented by the Fischer projection arbitrarily in use, thus obviating a need to reverse the Fischer representation.)



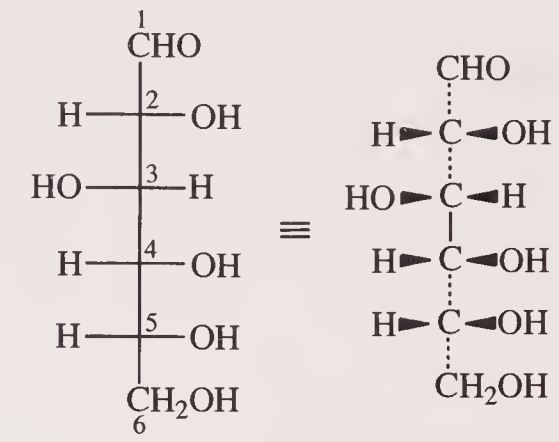
D-glyceraldehyde



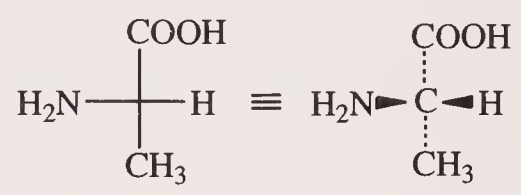
L-glyceraldehyde

For carbohydrates, in general, the position of the OH group attached to the highest-numbered carbon atom in the chain determines the assignment of D- and L-. For instance, in D-glucose the OH at position 5 is on the right-hand side of the Fischer projection.

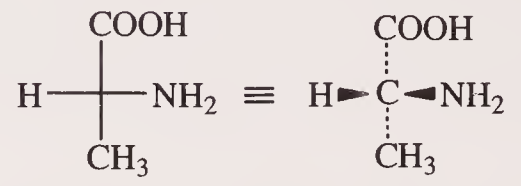
In α-amino acids, the L-compounds are those in which the NH_2 group is on the left-hand side of the Fischer projection in which the COOH group is at the top. Conversely, the D-compounds are those in which the NH_2 group is on the right-hand side.



D-glucose



L-alanine



D-alanine

D- and L- do *not* relate to the sign of rotation of an optically active molecule, which is designated (+)- or (–)- (formerly *d-* and *l-*)

The abbreviations D_s/L_s and D_G/L_G were formerly used in cases where there was potential ambiguity in assigning D/L configurations and refer to configuration relative to serine and glucose respectively (obsol.: use *R* and *S* conventions).

dansyl [[5-dimethylamino)-1-naphthalenyl]sulfonyl]

de- The prefix 'de-' followed by the name of a group or atom denotes replacement of that group or atom by hydrogen. Thus, in de-*N*-methylmorphine, the *N*-Me group of morphine has been replaced by *N*-H. Sometimes used in steroid nomenclature to denote the loss of an entire ring as in de-*A*-cholestane. 'Des-' is sometimes used instead of 'de-'

deca Multiplicative prefix denoting '10'. Undeca denotes '11' dodeca denotes '12', trideca denotes '13', etc.

decanoyl (1-oxodecyl) $H_3C(CH_2)_8CO–$

deci Numerical prefix denoting '10'. Used only in ring assembly names. Undeci denotes '11', dodeci denotes '12', trideci denotes '13', etc.

dehydro Loss of two hydrogen atoms from a compound designated by a trivial name can be denoted by the prefix 'didehydro'. Thus, 7,8-didehydrocholesterol is cholesterol with an additional double bond between atoms 7 and 8. In common usage, 'dehydro' is sometimes used instead of 'didehydro'. Dehydro can also mean removal of water, e.g. dehydromorphine

dendrimer Highly branched oligo- and polymeric compounds formed by reiterative reaction sequences. Also called starburst dendrimers, cascade molecules and arborols

Tomalia, D. A., *et al.*, *Angew. Chem., Int. Ed. Engl.*, 1990, 29, 138 (rev)

deoxy Denotes replacement of a hydroxy group by a hydrogen atom

depsides Esters formed from two or more molecules of the same or different phenolic acids

depsipeptides Compounds containing amino acids and hydroxy acids (not necessarily α-hydroxy acids) and having both ester and peptide bonds

des- See *de-*

desyl (2-oxo-1,2-diphenylethyl) PhCOCHPh–

deuterio D- Denotes replacement of a hydrogen atom by a deuterium atom. 'Deutero' is also used

dextro Denotes a compound which, in solution, rotates the plane of plane-polarised light to the right, Equivalent to (+)- or *d*-

di Numerical prefix denoting 'two'

diazene HN=NH Introduced relatively recently as a parent to simplify the nomenclature of azo compounds

diazeno diazenyl HN=N–

diazo N_2= Thus, diazomethane is H_2CN_2. 'Diazo compounds' are compounds containing the diazo group, R_2CN_2. The term 'diazo' has also been used in naming compounds RN=NX; for example, benzenediazohydroxide is PhN=NOH, benzenediazocyanide is PhN=NCN and benzenediazosulfonic acid is $PhN{=}NSO_3H$

diazoate Metal diazoates are compounds with the formula RN=N–OM (M = metal). Thus, PhN=NONa is sodium benzenediazoate

diazonio N_2^+–

-diazonium Ions RN_2^+ are named by adding the suffix 'diazonium' to the name of the parent substance RH. Thus, $PhN_2^+Cl^-$ is benzenediazonium chloride.

dicta Numerical prefix denoting '200'

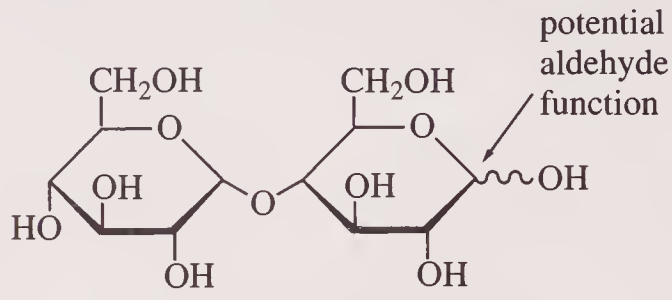
didehydro See *dehydro*

diimide diazene HN=NH

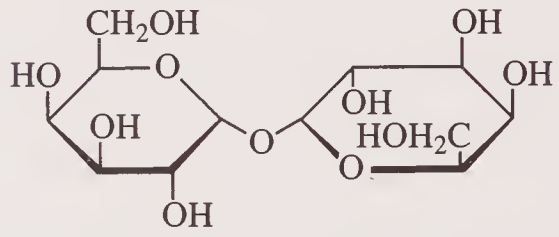
dinor See *nor*

dioxy –OO– Used when the free valencies are attached to different atoms that are not otherwise connected. Also called *epidioxy*. cf. *epoxy*

disaccharide A sugar produced where a glycoside of one monosaccharide is formed by another monosaccharide. Where the resulting sugar has a (potentially) free aldehyde function, it is called a reducing disaccharide, and where both aldehyde functions are involved in the linkage (1→1) glycoside, it is a non-reducing disaccharide



maltose (4-*O*-α-D-glucopyranosyl-D-glucose), a reducing disaccharide



α-D-galactopyranosyl α-D-galactopyranoside, a non-reducing disaccharide

diterpenoids Terpenoids having a C_{20} skeleton. For a comprehensive treatment of diterpenoids, see the *Dictionary of Natural Products*

dithio –SS– Usually used when the free valencies are attached to different atoms that are not otherwise connected

dithioacetals Sulfur analogues of acetals $R_2C(SR_2)$ (R is the same or different)

dl- Denotes a racemic mixture (*d-* + *l-*) (avoid: use (±)-)

DL- Denotes a racemic mixture (D- + L-) (avoid except for carbohydrates: use (±)-)

dodeca Numerical prefix denoting '12'

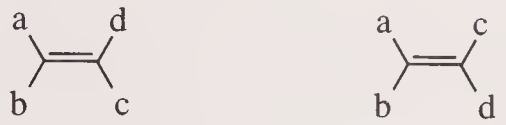
dodecanoyl (1-oxododecyl) $H_3C(CH_2)_{10}CO$–

duryl (2,3,5,6-tetramethylphenyl)

durylene (2,3,5,6-tetramethyl-1,4-benzenediyl)

E A stereochemical descriptor used to describe the configuration about a double bond. Usually

equivalent to *trans*-. In the following diagram, 'a' is a group or atom that takes precedence over atom or group 'b' using the sequence rule; similarly, 'c' takes precedence over 'd'.

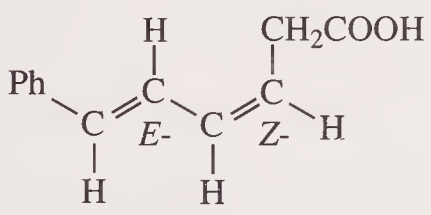


(*E*)- (*Z*)-

In DOC 6, line formulae are given for simple alkenes, where there is no possibility of confusion between (*E*)- and (Z)-, for example $H_3CCH_2CH{=}CHCH_3$, (*E*)- = *trans* and (*Z*)- = *cis*. Where there is any possibility of confusion, a two-dimensional structure diagram is shown.

For many compounds with more than one double bond, CAS cites (*E*)- and (*Z*)- without locants. The (*E*) and (*Z*) descriptors are cited in descending order of seniority. The most senior double bond is that which has the highest-ranking (sequence rule) substituent attached. Thus, the stereochemistry of the compound below is described as (*E,Z*)- because the phenyl group is the highest-ranked substituent attached to a doubly bonded atom

Blackwood, J. E., *et al.*, *J. Chem. Doc.*, 1968, **8**, 32



(*E,Z*)-

e- Equivalent to *E*- to denote configuration at a single bond with restricted rotation (*Beilstein*)

-ecane, -ecin, -ecine Hantzsch–Widman stems for 10-membered heterocyclic rings. See *Hantzsch–Widman names*

eicosa or **icosa** Numerical prefix denoting '20'. IUPAC recommend icosa; CAS use eicosa. DOC gives both, with eicosa preferred in entry names

eicosanoids See *icosanoids*

enamines Vinylic amines containing the unit N–C=C–. 'Enamino' is a general term for a radical derived from an enamine by removal of a hydrogen from the nitrogen atom

enanthoyl or **enanthyl** (1-oxoheptyl) $H_3C(CH_2)_5CO$-

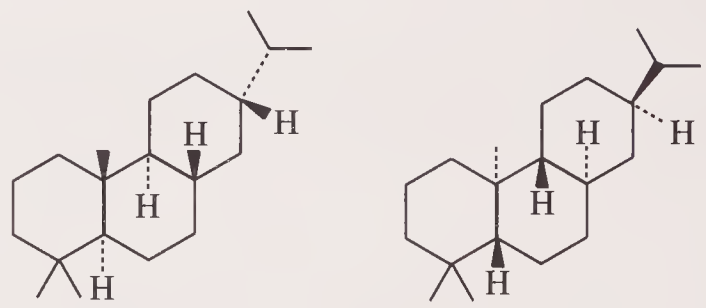
endo- Stereochemical descriptor used for bridged bicyclic systems. In a bicyclo[*X.Y.Z*] compound ($X \geq Y > Z$), 'exo-' denotes that a substituent on an *X* or *Y* bridge is on the opposite side of the molecule from the *Z* bridge. For a diagram, see *anti*-. Also, *endo* is used to indicate the insertion of an amino acid residue into a peptide chain; see *peptides*

***endo*-bond** A bond within a ring

-ene Usually denotes the presence of a double bond

enols Vinylic alcohols, tautomeric with aldehydes and ketones, containing the unit HO–C=C

ent- The prefix *ent*- (a contracted form of *enantio*-) denotes configurational inversion of all the asymmetric centres whose configurations are implied in a name. See the *Dictionary of Natural Products* for many examples. *enantio*- is used to designate a trivially named peptide in which the configurations of all the amino acid residues are the opposite to those in the naturally occurring compound



abietane *ent*-abietane

-epane Hantzsch–Widman stem for a seven-membered saturated heterocyclic ring not containing nitrogen

epi (greek 'upon') In carbohydrate chemistry, denotes an isomer differing in configuration at the α-carbon. Generally, to denote the opposite configuration at a chiral centre (e.g. 4-epiabietic acid). Also denotes a1,6-disubstituted napthalene (obsol.)

epidioxy, epidithio –OO– and –SS– Usually used when the free valencies are attached to different atoms that are otherwise connected

epimino –NH– Usually used when the free valencies are attached to different atoms that are otherwise connected

-epin, -epine Hantzsch–Widman stems for seven-membered heterocyclic rings. See *Hantzsch–Widman names*

episeleno, epithio –Se– and –S– Usually used when the free valencies are attached to different atoms that are otherwise connected

epoxides Cyclic ethers. Usually restricted to three-membered cyclic ethers (oxiranes)

epoxy –O– Used when the free valencies are attached to different atoms that are otherwise connected

epoxyimino, epoxynitrilo, epoxythio, epoxythioxy –O–NH–, –O–N=, –O–S– and –O–S–O– Used as bridges in naming bridged fused ring systems

erythro- A configurational prefix. See *carbohydrates*. It is used generally to denote compounds having the erythrose-like configuration (ambiguity can arise)

esters Compounds derived by condensation of an acid with an alcohol (or a phenol or thiol). The name of an ester consists of two parts, one derived from the alcohol and one derived from the acid. Thus, ethyl acetate is the ester from ethanol and acetic acid. Sometimes the alcohol information is given after the name of the acid as in 'acetic acid ethyl ester'.

CA indexing of esters. In *Chemical Abstracts*, esters are usually indexed at the name of the component acid. However, esters of some very common acids ('class I' acids) are indexed at the names of the component alcohol/phenol or thiol unless the alcohol/phenol or thiol component is also very common (a 'class I' alcohol).

Table 8.5 lists the 'class I' acids. All other acids are 'class II' acids.

Table 8.6 lists the 'class I' alcohols and phenols. The list of 'class I' thiols is completely analogous to the 'class I' alcohol list.

Table 8.5 'Class I' acids

acetic acid	methylcarbamic acid
aminobenzoic acid (all isomers)	nitric acid
benzenesulfonic acid	nitrobenzoic acid (all isomers)
benzoic acid	phenylcarbamic acid
boric acid (H_3BO_3)	phosphinic acid
carbamic acid	phosphonic acid
carbonic acid	phosphoric acid
dinitrobenzoic acid (all isomers)	phosphorodithioic acid
formic acid	phosphorothioic acid
methanesulfonic acid	phosphorous acid
4-methylbenzenesulfonic acid	propanoic acid
	sulfuric acid
	sulfurous acid

Table 8.6 'Class I' alcohols/phenols

benzeneethanol	1-hexanol
benzenemethanol	methanol
1-butanol	methylphenol (all isomers)
2-butanol	2-methyl-1-propanol
chlorophenol (all isomers)	2-methyl-2-propanol
cyclohexanol	nitrophenol (all isomers)
1-decanol	1-nonanol
2-(diethylamino)ethanol	1-octadecanol
2-(dimethylamino)ethanol	1-octanol
1-dodecanol	1-pentanol
ethanol	phenol
ethenol	1-propanol
2-ethyl-1-butanol	2-propanol
2-ethyl-1-hexanol	2-propen-1-ol
1-heptanol	

The following combinations occur:

Acid	Alcohol	Indexed at
1. class I	class I	acid
2. class I	class II	alcohol
3. class II	class I	acid
4. class II	class II	acid

Examples of each of these combinations:

1. Methyl acetate is indexed at 'Acetic acid, methyl ester'.
2. Chloromethyl acetate is indexed at 'Methanol, chloro-, acetate.
3. Methyl chloroacetate is indexed at 'Acetic acid, chloro-, methyl ester'.
4. Chloromethyl chloroacetate is indexed at Acetic acid, chloro-, chloromethyl ester'.

There is one exception. Where a polybasic 'class I' acid, e.g. phosphoric acid, is esterified by two or more different alcohols, the acid heading is always used. Thus, chloromethyl dimethyl phosphate is indexed at 'Phosphoric acid, chloromethyl dimethyl ester' because the alcoholic components are unlike.

-etane, -ete, -etene Hantzsch–Widman stems for four-membered heterocyclic rings. See *Hantzsch–Widman names*

ethano $-CH_2-CH_2-$ Used as a bridge in naming bridged fused ring systems

etheno –CH=CH– Used as a bridge in naming bridged fused ring systems

ethenyl H_2C=CH–

ethenylidene H_2C=C=

ethers Compounds R^1OR^2. The word 'ether' is used in radicofunctional nomenclature. Thus, diethyl ether is Et_2O (sometimes called ethyl ether), methyl phenyl ether is MeOPh, and ethylene glycol monomethyl ether is $MeOCH_2CH_2OH$

ethiodide, ethobromide, ethochloride Denotes a base quaternised with ethyl iodide, ethyl bromide or ethyl chloride

ethoxalyl (ethoxyoxoacetyl) EtO_2CCO–

ethoxide The anion EtO^-. Thus, sodium ethoxide is EtONa

ethoxy EtO–

(ethoxycarbonyl) EtO_2C–

ethyl H_3CCH_2– Often abbreviated to Et in structural and line formulae. In DOC 6, Et is used only for ethyl groups attached to heteroatoms

ethylene As a radical name, 'ethylene' has been used for the diradical 1,2-ethanediyl $–CH_2CH_2–$

(ethylenedioxy) $–OCH_2CH_2O–$

ethylidene H_3CCH=

ethylidyne $H_3CC{\equiv}$

(ethylthio) EtS–

ethynyl HC≡C–

-etidine, -etine Hantzsch–Widman stems for four-membered heterocyclic rings. See *Hantzsch–Widman names*

etio (aetio) (Greek *aitia*, 'cause') Denotes a degradation product, e.g. Etiocholanic acid

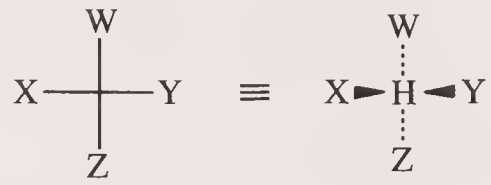
***exendo*-bond** A bond that is directly attached to a ring and within another ring

***exo*-** (Greek 'outside') Stereochemical descriptor used for bridged bicyclic systems. In a bicyclo[*X.Y.Z*] compound ($X \geq Y > Z$), *exo-* denotes that a substituent on an *X* or *Y* bridge is on the same side of the molecule as the *Z* bridge. For a diagram, see *anti-*

***exo*-bond** A bond directly attached to a ring

fatty acids Carboxylic acids derived from animal or vegetable fat or oil. The term is sometimes used to denote all acyclic aliphatic carboxylic acids

Fischer projection A method of representing asymmetric carbon atoms.



By convention, the atoms or groups attached to the horizontal bonds (X, Y) are considered to be above the plane of the paper and those attached to the vertical bonds (W, Z) are below the plane of the paper. *Caution*: Rotating a Fischer projection by 90° inverts the stereochemistry!

flavonoids A large group of natural products that are widespread in higher plants, derived by cyclisation of a chalcone precursor. Entries for a limited selection of the most important flavonoids are given in DOC 6. For a comprehensive treatment of flavonoids, see the *Dictionary of Natural Products*

fluoride The word 'fluoride' is used in radicofunctional names such as methyl fluoride (MeF) and benzoyl fluoride (PhCOF). It is also used in additive names such as ethylene difluoride (FCH_2CH_2F)

fluoro F–

fluoryl O_2F–

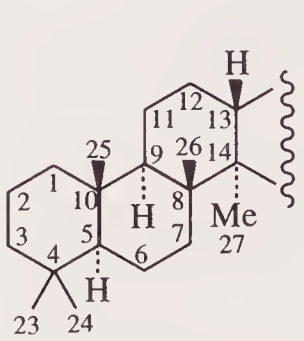
formamido (formylamino) HCONH–

formazyl [(phenylazo)(phenylhydrazonyl)methyl] PhN=NC(=NNHPh)–

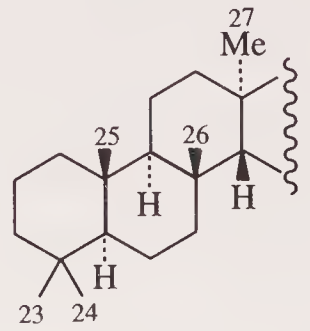
formimidoyl (iminomethyl) HN=CH–

formyl O=CH–

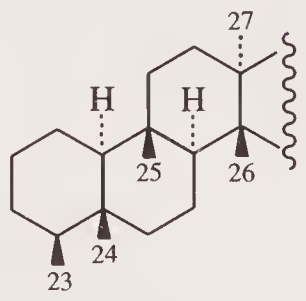
***friedo*-** In a triterpene name, *friedo-* denotes that a methyl group has migrated from one position to



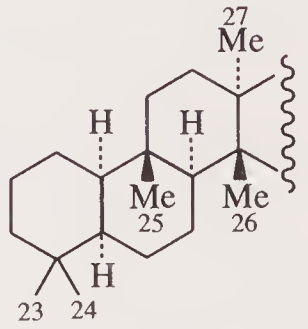
normal triterpene



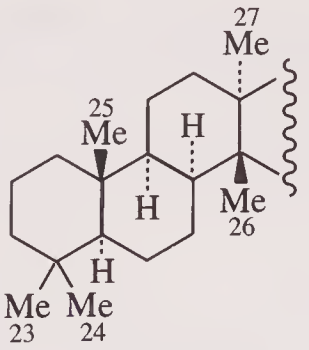
D-*friedo*-



D:A-friedo-



D:B-friedo-



D:C-friedo-

another. For many examples see the *Dictionary of Natural Products*

fulminate An ester of fulminic acid (HONC). Thus, methyl fulminate is MeONC

fumaroyl (*E*)-(1,4-dioxo-2-butene-1,4-diyl) –COCH=CHCO– The (*Z*)-form is 'maleoyl'

functional group A group characterised by the presence of heteroatoms and/or unsaturation, which can take part in chemical reactions, e.g. –COOH, –SH

functional replacement nomenclature A type of nomenclature most commonly used in naming phosphorus and arsenic compounds. For details see *phosphorus compounds*

furanoses Cyclic acetal or hemiacetal forms of saccharides in which the ring is five-membered. See *carbohydrates*

-furanoside Denotes a glycoside containing a furanose ring. See *glycoside*

-furanosyl Denotes a radical derived from a furanose by detaching the anomeric OH group

furfural As a radical name, 'furfural' denotes (2-furanylmethylene). 'Furfural' usually refers to 2-furancarboxaldehyde

furfuryl (2-furanylmethyl)

furfurylidene (2-furanylmethylene)

furo The ring fusion prefix from furan

furoyl (furanylcarbonyl)

furyl A contracted form of furanyl

fused ring systems See *ring fusion names*

galacto- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

galloyl (3,4,5-trihydroxybenzoyl) $3,4,5\text{-}(HO)_3C_6H_2CO–$

gem An abbreviation of *geminal.* Used to denote that two groups are attached to the same atom as in *gem*-diol and *gem*-dimethyl groups

gentisoyl (2,5-dihydroxybenzoyl) $2,5\text{-}(HO)_2C_6H_3CO–$

germa Replacement prefix denoting germanium. For a full coverage of organogermanium compounds, see the *Dictionary of Organometallic Compounds*

gluco A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

glucosinolates Mustard oil glycosides. See the *Dictionary of Natural Products*

glutaminyl $H_2NCO(CH_2)_2CH(NH_2)CO–$ The acyl radical from glutamine used in naming peptides

α-glutaminyl $H_2NCOCH(NH_2)CH_2CH_2CO–$ The acyl radical from α-glutamine used in naming peptides

glutamoyl $–CO(CH_2)_2CH(NH_2)CO–$ The diacyl radical from glutamic acid

glutamyl This could mean either glutamoyl or an unspecified glutamyl radical

α-glutamyl $HOOC(CH_2)_2CH(NH_2)CO–$ An acyl radical from glutamic acid used in naming peptides

γ-glutamyl $HOOCCH(NH_2)(CH_2)_2CO–$ An acyl radical from glutamic acid used in naming peptides

glutaryl (1,5-dioxo-1,5-pentanediyl) $–CO(CH_2)_3CO–$

glycals Olefinic sugars with a double bond between positions 1 and 2

glycans Polysaccharides made up of monosaccharide units linked glycosidically

glycaric acids Another name for aldaric acids

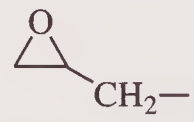
glycerides Esters of glycerol with fatty acids

glycero- A configurational prefix. See *carbohydrates*

glyceroyl (2,3-dihydroxy-1-oxopropyl) $HOCH_2CH(OH)CO–$

glyceryl 1,2,3-propanetriyl $–CH(CH_2–)_2$

glycidyl oxiranylmethyl



glyco(l)loyl or glyco(l)lyl (hydroxyacetyl) $HOCH_2CO–$

glycols Diols. For example, ethylene glycol is $HOCH_2CH_2OH$ and propylene glycol is $H_3CCH(OH)CH_2OH$

glycopeptides, glycoproteins Substances in which

a carbohydrate component is linked to a peptide or protein

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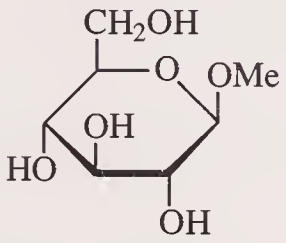
glycoside A mixed acetal resulting from the replacement of the hydrogen atom on the anomeric (glycosidic) OH of the cyclic form of a sugar by a radical R derived from an alcohol or phenol (ROH). They are named by changing the terminal '-e' of the name of the corresponding cyclic form of the saccharide by '-ide'; the name of the R radical is put at the front of the name followed by a space.



methyl β-D-glucopyranoside

Many thousand of naturally occurring glycosides are known: see the *Dictionary of Natural Products*

glycosyl A radical formed when the hemiacetal OH group is detached from the cyclic form of an aldose or ketose

glycyl (aminoacetyl) $H_2NCH_2CO–$ Used in naming peptides

glyoxalinyl or **glyoxalyl** imidazolyl

glyoxyloyl or **glyoxylyl** (oxoacetyl) OHCCO–

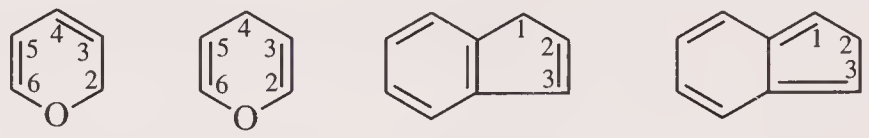
guanidino [(aminoiminomethyl)amino] $H_2NC(=NH)NH–$

guanyl (aminoiminomethyl) $H_2NC(=NH)–$

gulo- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

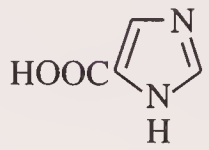
H An italic H appearing with the name of a ring or ring system usually denotes an indicated or added hydrogen atom.

Indicated hydrogen. For some fused polycyclic ring systems and certain monocyclic heterocycles that contain the maximum number of cumulative double bonds, it is possible to have more than one isomer; these isomers differ in the positions of the double bonds. They are distinguished by using *H* with the appropriate locant to indicate that atom which is not connected to either neighbouring ring atom by a double bond. The *H* is known as indicated hydrogen.



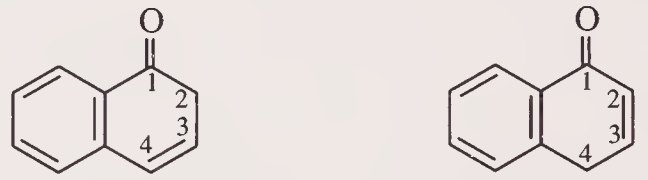
2*H*-pyran 4*H*-pyran 1*H*-indene 2*H*-indene

Indicated hydrogen has the highest priority in naming compounds. Thus



is 1*H*-imidazole-5-carboxylic acid and not 3*H*-imidazole-4-carboxylic acid

Added hydrogen. Sometimes a hydrogen atom needs to be added to a ring system in order to accommodate structural features such as principal groups. This is called added hydrogen. For example, introduction of a ketone group into naphthalene will mean the removal of one double bond and there will then be a CH_2 unit in the ring. The position of this CH_2 unit is indicated by using *H* with the appropriate locant.



1(2*H*)-naphthalenone 1(4*H*)-naphthalenone

Residual hydrogen. In almost completely halogenated compounds, the positions of the residual hydrogens is sometimes indicated by *H*. Thus, 1*H*,4*H*-decafluoropentane is $HCF_2CF_2CF_2CHFCF_3$

halo A general term for a monovalent substituent derived from a halogen atom, i.e. F–, Cl–, Br–, I–

halohydrins Halo alcohols. For example, ethylene bromohydrin is $BrCH_2CH_2OH$

Hantzsch–Widman names Hantzsch–Widman names are used for some one-ring heterocyclic systems that do not have trivial names. The names are applied to monocyclic compounds containing one or more heteroatoms in three- to ten-membered rings. The names are derived by combining the appropriate prefix or prefixes for the heteroatoms with a stem denoting the size of the ring (see below). The state of hydrogenation is indicated either in the stem or by the prefixes 'dihydro', 'tetrahydro', etc.

The prefixes are the normal replacement prefixes (see *Replacement nomenclature*), although

Table 8.7 Original Hantzsch–Widman stems

No. of members in ring	Rings containing nitrogen		Rings containing no nitrogen	
	Unsatn.	Satn.	Unsatn.	Satn.
3	-irine	-iridine	-irene	-irane
4	-ete	-etidine	-ete	-etane
5	-ole	-olidine	-ole	-olane
6	-ine	–	-in	-ane
7	-epine	–	-epin	-epane
8	-ocine	–	-ocin	-ocane
9	-onine	–	-onin	-onane
10	-ecine	–	-ecin	-ecane

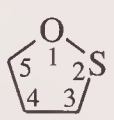
elision of the final 'a' often occurs. The prefixes are cited in the following order; fluora, chlora, broma, ioda, oxa, thia, selena, tellura, aza, phospha, arsa, stiba, bisma, sila, germa, stanna, plumba, bora, mercura. *Chemical Abstracts* does not use Hantzsch–Widman names for rings containing silicon.

The stems used originally (*Nomenclature of Organic Chemistry*, p. 53) are as shown in Table 8.7.

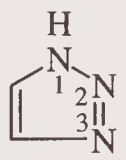
The stems for unsaturated rings imply the maximum possible number of non-cumulative double bonds. Rings with more than 10 members are named by replacement nomenclature, e.g. aza-cycloundecane.

oxirene

aziridine



1,2-oxathiolane



1*H*-1,2,3-triazole

Several exceptions to the original rules were made in order to avoid confusion with other compounds; for example, phosphorine was used instead of phosphine. In order to avoid such exceptions, the extended Hantzsch–Widman system (*Pure Appl. Chem.*, 1983, **55**, 409) was introduced. This uses the stems shown in Table 8.8.

Some common monocyclic hetero systems have trivial names, for example, pyridine and furan.

In the case of four- and five-membered rings, special stems were once used for the structures containing one double bond where there can be more than one double bond. These stems are: '-etine' for four-membered rings containing nitrogen, '-etene' for four-membered rings containing no nitrogen, '-oline' for five-membered rings containing nitrogen, and '-olene' for five-membered rings containing no nitrogen. These stems are no longer recommended.

Table 8.8 Extended Hantzsch–Widman stems[a]

No. of members in ring[b]	Unsaturation	Saturation
3	-irene	-irane
4	-ete	-etane
5	-ole	-olane
6A	-ine	-ane
6B	-ine	-inane
6C	-inine	-inane
7	-epine	-epane
8	-ocine	-ocane
9	-onine	-onane
10	-ecine	-ecane

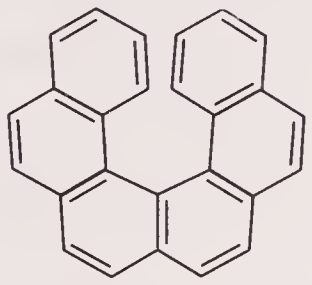
[a] The stem for the least preferred heteroatom is selected.
[b] 6A applies to rings containing: O, S, Se, Te, Bi, Hg.
6B applies to rings containing: N, Si, Ge, Sn, Pb.
6C applies to rings containing: B, F, Cl, Br, I, P, As, Sb.

Δ^2-azetine or 2-azetine

Haworth representation A method of representing monosaccharides in their cyclic hemiacetal form. See *carbohydrates*

hecta Numerical prefix denoting '100'

helicenes Ortho-fused polycyclic aromatic compounds that have a helical structure



hexahelicene

hemi Numerical prefix denoting 'a half'

hemiacetal A compound with formula $R^1CH(OH)OR^2$ or $R^1R^2C(OH)OR^3$

hemicarcerand A bow-shaped molecule capable of complexing small molecules in its cavity. See *carcerand*

hemiketal A hemiacetal derived from a ketone

hemimercaptals, hemimercaptoles Compounds $R^1R^2C(SH)(SR^3)$

hendeca Numerical prefix denoting '11'

heneicosa or **henicosa** Numerical prefix denoting '21'. CAS uses heneicosa; IUPAC recommends henicosa. Similarly, hentriaconta denotes '31', hentetraconta denotes '41', etc.

hepta Numerical prefix denoting 'seven'. Heptaconta denotes '70' heptacosa denotes '27', and heptadeca denotes '17'

heptadecanoyl (1-oxoheptadecyl) $H_3C(CH_2)_{15}CO–$

heptanoyl (1-oxoheptyl) $H_3C(CH_2)_5CO–$

heptitol An alditol with seven carbon atoms

heptonic acid An aldonic acid with seven carbon atoms

heptose An aldose with seven carbon atoms

heptulose A ketose with seven carbon atoms

hetero (Greek *heteros*, 'other') Prefix meaning 'different', e.g. heteroxanthine, heterocycle

hexa Numerical prefix denoting 'six'. Hexaconta denotes '60', hexacosa denotes '16', and hexadeca denotes '26'

hexadecanoyl (1-oxohexadecyl) $H_3C(CH_2)_{14}CO–$

hexakis Multiplicative prefix used instead of hexa with complex terms and to avoid ambiguity

hexamethylene 1,6-hexanediyl $–CH_2)_6–$

hexanoyl (1-oxohexyl) $H_3C(CH_2)_4CO–$

hexitol An alditol with six carbon atoms

hexopyranose A hexose in the pyranose form

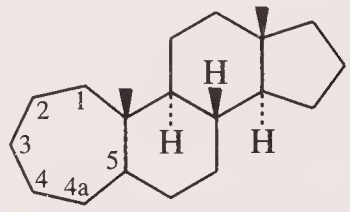
hexose An aldose with six carbon atoms

hexulose A ketose with six carbon atoms

hippuroyl or **hippuryl** *N*-benzoylglycyl $PhCONHCH_2CO–$

histidyl The acyl radical derived from histidine used in naming peptides

homo Denotes incorporation of CH_2 as an additional member in a ring in a steroid or a terpene; also for example in homophthalic acid



A-homoandrostane

homoallyl 3-butenyl $H_2C=CHCH_2CH_2–$

homocysteinyl $HS(CH_2)_2CH(NH_2)CO–$ The acyl radical from homocysteine used in naming peptides

homoseryl $HO(CH_2)_2CH(NH_2)CO–$ The acyl radical from homoserine used in naming peptide

hydrazi –NHNH–

hydrazide A compound formed by the replacement of the hydroxy group of an acid by $–NHNH_2$. Thus, acetohydrazide is $H_2CCONHNH_2$ and benzenesulfonohydrazide is $PhSO_2NHNH_2$

hydrazidines Compounds $RC(=NNH_2)NHNH_2$. The term has also been applied to $RC(=NH)NHNH_2$, $RC(=NH)NH_2$ and $RC(NH_2)=NN=C(NH_2)R$

hydrazino $H_2NNH–$

hydrazo –NHNH– Usually used when the free valencies are attached to different atoms that are usually otherwise connected. 'Hydrazo compounds' are compounds RNHNHR. For example, hydrazobenzene is PhNHNHPh

hydrazone A compound derived from an aldehyde or ketone by replacement of the carbonyl oxygen by $=NNH_2$. Thus, acetone hydrazone is $(H_3C)_2C=NNH_2$

hydrazonic acids Compounds $RC(=NNH_2)OH$

hydrazono $H_2NN=$

-hydrazonyl Suffix denoting a radical formed by loss of OH from a hydrazonic acid

hydro Denotes an added hydrogen atom. Thus, 'dihydro' denotes saturation of one double bond

hydrocinnamoyl (1-oxo-3-phenylpropyl) $PhCH_2CH_2CO–$

hydrocinnamyl (3-phenylpropyl) $Ph(CH_2)_3$–

hydrodisulfides Compounds RSSH

hydrogen The word 'hydrogen' is used to indicate an acid salt or ester of a dibasic acid. Thus, potassium hydrogen heptanedioate is $HOOC(CH_2)_5COOK$

hydroperoxides Compounds ROOH. Thus, ethyl hydroperoxide is EtOOH

hydroperoxy HOO–

hydroseleno HSe–

hydrosulfides Old name for thiols. Thus, ethyl hydrosulfide is EtSH

hydroxamamides Another name for amidoximes

hydroxamic acids Compounds RC(O)NHOH

hydroxamino (hydroxyamino) HONH–

hydroximic acids Compounds RC(=NOH)OH

hydroximino (hydroxyimino) HONH=

-hydroximoyl Suffix denoting an acyl radical formed by removal of OH from a hydroximic acid

hydroxy HO–

hydroxylamine H_2NOH

hygroyl (1-methylprolyl)

hypo (Greek 'under') Indicates a lower state of oxidation, e.g. hypoxanthine

hypochlorite A salt or ester of hypochlorous acid (HOCl). Thus, methyl hypochlorite is MeOCl

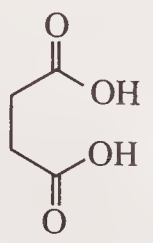
i- An abbreviation for 'inactive' as in *i*-tartaric acid (obsol.). Also for iso- as an *i*-pentane (obsol.)

icosa or **eicosa** Numerical prefix for '20'. CAS uses eicosa; IUPAC recommends icosa

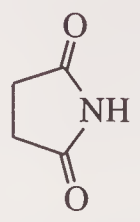
icosanoids Unsaturated C_{20} fatty acids and related compounds such as leukotrienes

ido- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

imides A class of compounds derived by replacement of two OH groups of a dibasic acid by –NH– or –N(R)–.



succinic acid



succinimide

Also 'imide' is used to indicate addition of =NH at a heteroatom as in phosphine imide $H_3P{=}NH$

imidic acids Compounds RC(=NH)OH

-imido Suffix denoting a radical formed from an imide by removal of the hydrogen from the imide nitrogen as in succinimido

imidocarbonyl carbonimidoyl –C(=NH)–

imidogen HN:, a neutral monovalent nitrogen species

-imidoyl Suffix denoting a radical formed by removal of OH from an imidic acid

imines Compounds $R^1R^2C{=}NH$. They can be named by adding the suffix '-imine' either to a parent name or to an '-ylidene' radical. Thus, $H_3C(CH_2)_4CH{=}NH$ is 1-hexanimine or hexylidenimine

iminio $H_2N^+{=}$

imino HN=

-in Hantzsch–Widman stem for a six-membered fully unsaturated heterocyclic ring not containing nitrogen, such as dioxin

-inane Hantzsch–Widman stem for some six-membered heterocyclic rings. See *Hantzsch–Widman names*

indicated hydrogen See *H*

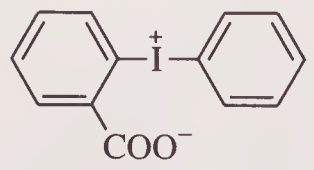
indyl A contracted form of indolyl

-ine Hantzsch–Widman stem for some six-membered fully saturated heterocyclic ring containing nitrogen, as in oxazine

-inine Hantzsch–Widman stem for some six-membered heterocyclic rings. See *Hantzsch–Widman names*

-inium Denotes a positively charged species derived from a base with a name ending in -ine. Thus, anilinium is $PhNH_3^+$

inner salts *Chemical Abstracts* consider compounds such as betaines to be formed by the loss of water from the corresponding hydroxides and name them by use of the expression 'hydroxide, inner salt'.



(2-carboxyphenyl)phenyliodonium, hydroxide, inner salt

inosamines Aminodeoxyinositols, i.e. 6-amino-1,2,3,4,5-cyclohexanepentols

inositols 1,2,3,4,5,6- cyclohexanehexols The various isomers are designated with the prefixes *allo-, chiro-, cis-, epi-, muco-, myo-, neo-* and *scyllo-*. For the structures, see DOC 6. For further details of the nomenclature, including assignment of stereochemistry, see *Biochem. J.,* 1976, **153**, 25

inososes 2,3,4,5,6-pentahydroxycyclohexanones

inseparable prefix One that forms an inseparable, therefore indexable, part of a name, e.g. iso- in isopropyl. The tendency in modern nomenclature is towards such prefixes becoming inseparable

iodide The word 'iodide' is used in radicofunctional names such as methyl iodide (MeI) and benzoyl iodide (PhCOI)

iodo I

iodonio HI^+–

iodonium H_2I^+

iodoso iodosyl OI–

iodosyl OI–

iodoxy iodyl O_2I–

iodyl O_2I–

-irane, -irene, -iridine, -irine Hantzsch–Widman stems for three-membered heterocyclic rings. See *Hantzsch–Widman names*

iso Prefix denoting isomerism, especially carbon chain branching (isohexanoic acid = 4-methylpentanoic acid). In the old literature it can be treated as a separable prefix, e.g. *iso*-propyl; in the modern literature usually and in DOC 6 always it is treated as an inseparable prefix, e.g. isopropyl

isoallyl 1-propenyl $H_3CCH{=}CH$–

isoamyl (3-methylbutyl) $(H_3C)_2CHCH_2CH_2$–

isobutenyl (2-methyl-1-propenyl) $(H_3C)_2C{=}CH$–

isobutoxy (2-methylpropoxy) $(H_3C)_2CHCH_2O$–

isobutyl (2-methylpropyl) $(H_3C)_2CHCH_2$– Often abbreviated to Bu^i ir i-Bu in structural and line formulae

isobutylidene (2-methylpropylidene) $(H_3C)_2CHCH{=}$

isobutyryl (2-methyl-1-oxopropyl) $(H_3C)_2CHCO$–

isocrotyl (2-methyl-1-propenyl) $(H_3C)_2C{=}CH$–

isocyanates Compounds RNCO. Thus, methyl isocyanate is MeNCO

isocyanato OCN–

isocyanides Compounds RNC. Thus, methyl isocyanide is MeNC

isocyano CN–

isohexyl (4-methylpentyl) $(H_3C)_2CH(CH_2)_3$–

isoleucyl $H_3CCH(CH_3)CH(NH_2)CO$–. The acyl radical from isoleucine used in naming peptides

isonicotinoyl (4-pyridinylcarbonyl)

isonitriles Isocyanides Compounds RNC

isonitro *aci*-nitro HON(O)=

isonitroso (hydroxyimino) HON= 'Isonitroso compounds' is an obsolete term for oximes

isopentyl (3-methylbutyl) $(H_3C)_2CHCH_2CH_2$–

isopentylidene (3-methylbutylidene) $(H_3C)_2CHCH_2CH{=}$

isophthaloyl 1,3-phenylenedicarbonyl $1,3\text{-}C_6H_4(CO{-})_2$

isoprenoids Compounds such as terpenes that are derived from isoprene units. Isoprene is 2-methyl-1,3-butadiene, $H_2C{=}C(CH_3)CH{=}CH_2$. See the *Dictionary of Natural Products*

isopropenyl (1-methylethenyl) $H_2C{=}C(CH_3)$–

isopropoxy (1-methylethoxy) $(H_3C)_2CHO$–

isopropyl (1-methylethyl) $(H_3C)_2CH$– Often abbreviated to Pr^i or i-Pr in structural and line formulae. In the old literature usually given as *iso*-Propyl (separable prefix)

isopropylidene (1-methylethylidene) $(H_3C)_2C{=}$

isoquino The ring fusion prefix derived from isoquinoline

isoquinolyl A contracted form of isoquinolinyl

isoselenocyanates Compounds RNCSe

isoselenocyanato SeCN–

isothiocyanates Compounds RNCS. Thus, methyl isothiocyanate is MeNCS

isothiocyanato SCN–

1-isoureido [(iminohydroxymethyl)amino] $HN{=}C(OH)NH$–

3-isoureido [(aminohydroxymethylene)amino] $H_2NC(OH){=}N$–

isovaleryl (3-methyl-1-oxobutyl) $(H_3C)_2CHCH_2CO$–

isovalyl $H_3CCH_2C(CH_3)(NH_2)CO$– The acyl radical from isovaline used in naming peptides

-itol Suffix denoting a polyalcohol as in alditol, cyclitol. See *alditols* and *cyclitols*

-ium Suffix denoting a positively charged species

ketals Acetals derived from ketones (obsol.)

ketazines Azines derived from ketones

ketene A general term for compounds $R^1R^2C{=}C{=}O$. When used for a specific compound, 'ketene' is ethenone, $H_2C{=}C{=}O$

keto oxo O= Now used only in a generic sense as in 'ketoesters'

ketones Compounds R^1COR^2. Usually named by use of the suffix '-one' or the prefix 'oxo'. Radicofunctional names are sometimes used. Thus, dimethyl ketone is H_3CCOCH_3 and ethyl methyl ketone is $H_3CCH_2COCH_3$

ketoses Monosaccharides containing a ketone group

ketoximes Oximes of ketones

kilia Numerical prefix denoting '1000'

l- An abbreviated form of *levo*- or *laevo* (obsol.)

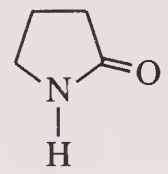
L- A configurational descriptor. See D-. For L_S and L_G, see under D- also

labelled compounds There are two main methods used for naming isotopically labelled compounds. For specifically labelled compounds IUPAC recommends forming the name by placing the nuclide symbols (plus locants if necessary) in square brackets before the name of the unlabelled compound or that part of the name which is isotopically modified.

Chemical Abstracts uses the Boughton system in which italicized nuclide symbols follow the name or part of the name of the unlabelled compound. The symbols *-d* and *-t* are used to denote deuterium and tritium, respectively

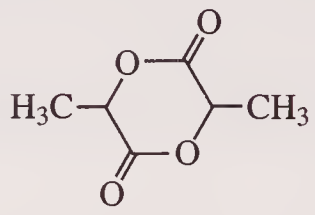
	CA	IUPAC
CH_2D_2	methane-d_2	[$^2H_2$]methane
$H_3C^{14}CH_2OH$	ethanol-*1*-^{14}C	[1-^{14}C]ethanol

lactams Compounds containing a group –CO–NH– as part of a ring. β-Lactams have four-membered rings, γ–lactams have five-membered rings, δ-lactams have six-membered rings, etc.



γ-butyrolactam or 4-butanelactam

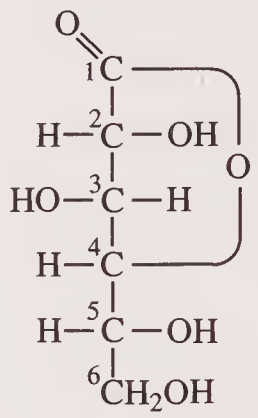
lactides Intramolecular cyclic esters formed by self-esterification from two or more molecules of a hydroxy acid



dilactide
(from lactic acid)

lactims Tautomers of lactams containing a group –C(OH)=N– as part of a ring

lactones Intramolecular cyclic esters of hydroxy acids. They contain a group –CO–O– as part of a ring. β-Lactones have four-membered rings, γ-lactones have five-membered rings, δ-lactones have six-membered rings, etc.



D-glucono-1,4-lactone

lactoyl (2-hydroxy-1-oxopropyl) $H_3CCH(OH)CO–$

laevo See *levo*-

lanthionyl $S[CH_2CH(NH_2)CO–]_2$

lauroyl (1-oxododecyl) $H_3C(CH_2)_{10}CO–$

lauryl dodecyl $H_3C(CH_2)_{11}$

leuco- (Greek 'white') Prefix denoting usually the reduced colourless form of a dye

leucyl $(H_3C)_2CHCH_2CH(NH_2)CO–$ The acyl radical from leucine used in naming peptides

levo- or ***laevo-*** Indicates a molecule that, in solution, rotates the plane of plane-polarised light to the left. Equivalent to (–)-. Abbreviated to *l*- (obsol.)

levulinoyl or **laevulinoyl** (1,4-dioxopentyl) $H_3CCOCH_2CH_2CO–$

lignans Plant products of low molecular weight formed primarily from oxidative coupling of two cinnamyl units. Lignins are natural polymers derived from lignans. For more information, see the *Dictionary of Natural Products*

lin- Denoting a linear arrangement of rings (obsol.)

lipids The term is applied to substances of biological origin that are soluble in hydrocarbons or ether. They include fats and oils, waxes, phospholipids and some steroids. For more information, see the *Dictionary of Natural Products*

lysyl $H_2N(CH_2)_4CH(NH_2)CO–$ The acyl radical from lysine used in naming peptides

lyxo- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

m- Abbreviation for *meta-*

macrolides Macrocyclic lactones

maleoyl (*Z*)-(1,4-dioxo-2-butene-1,4-diyl) $–COCH=CHCO–$ The (*E*)-form is 'fumaroyl'

maleyl (*Z*)-(3-carboxy-1-oxo-2-propenyl) $HOOCCH=CHCO–$

malonyl (1,3-dioxo-1,3-propanediyl) $–COCH_2CO–$

maloyl (2-hydroxy-1,4-dioxo-1,4-butanediyl) $–COCH_2CH(OH)CO–$

mandeloyl (hydroxyphenylacetyl) $PhCH(OH)CO–$

manno- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

menthyl A contracted form of menthanyl, the radical derived from menthane

mercaptals Dithioacetals

mercaptans An old name for 'thiols'. Thus, ethyl mercaptan is ethanethiol, EtSH

mercapto HS–

mercaptoles Mercaptals derived from ketones

mesaconoyl (*E*)-[2-methyl-1,4-dioxo-2-butene-1,4-diyl] $–COCH=C(CH_3)CO–$ The (*Z*)-form is 'citraconyl'

mesate A salt or ester of methanesulfonic acid ($MeSO_3H$)

mesidino [(2,4,6-trimethylphenyl)amino] $2,4,6\text{-}(H_3C)_3C_6H_2NH–$

mesityl (2,4,6-trimethylphenyl) $2,4,6\text{-}(H_3C)_3C_6H_2–$

α-mesityl [(3,5-dimethylphenyl)methyl] $3,5\text{-}(H_3C)_2C_6H_3CH_2–$

meso Denotes an internally compensated diastereoisomer of a chiral compound having an even number of chiral centres. For example, *meso*-tartaric acid contains two chiral centres of opposite chirality and is optically inactive. Also denotes the middle position of substitution, e.g. the 9 position in anthracene (obsol.)

mesoionic compounds Polyheteroatom five-membered ring betaines stabilised by electron delocalisation, having dipole moments not less than 5D and in which electrons and positive charge are delocalised over a part of the ring and attached groups, and in which electrons and a negative charge, formally on an α-atom (normally a hetero-atom) are delocalized over the remaining part of the ring. See *munchnones* and *sydnones*.
Cheung K. *et al*, *Acta Cryst. Sect. C.*, 1993, **49**, 1092

mesoxalo (caroxyoxoacetyl) $HOOCCOCO–$

mesoxalyl (1,2,3-trioxo-1,3-propanediyl) $–COCOCO–$

mesyl (methylsulfonyl) $MeSO_2–$

mesylate A salt or ester of methanesulfonic acid ($MeSO_3H$)

meta- Denotes 1,3-substitution on a benzene ring

metacyclophanes Cyclophanes in which the benzene rings are *meta*-substituted by the aliphatic bridging chains

metanilyl [3-aminophenyl)sulfonyl] $3\text{-}H_2NC_6H_4SO_2–$

methacryloyl (2-methyl-1-oxo-2-propenyl) $H_2C=C(CH_3)CO–$

methallyl (2-methyl-2-propenyl) $H_2C=C(CH_3)CH_2–$

methanetetrayl =C=

methano $–CH_2–$ Used as a bridge name in bridged fused cyclic systems

methenyl methylidyne HC≡

methine The group =C– is sometimes referred to as the 'methine' group

methiodide Indicates a base that has been quaternised with methyl iodide

methionyl $MeSCH_2CH_2CH(NH_2)CO–$ The acyl radical from methionine used in naming peptides

methobromide, methochloride Indicates a base quaternised with methyl bromide or methyl chloride. Other variants, such as metho-*p*-toluene-sulfonate, are also used

methoxalyl (methoxyoxoacetyl) $MeO_2COCO–$

methoxy MeO–

(methoxycarbonyl) MeO_2C–

methyl H_3C– Often denoted by Me in structural and line formulae. (In DOC, Me is used only for methyl groups attached to heteroatoms)

methylene H_2C= or $–CH_2–$ Trimethylene is $–CH_2CH_2CH_2–$, tetramethylene is $–CH_2CH_2CH_2CH_2–$, etc.

(methylenedioxy) $–OCH_2O–$

methylidene methylene H_2C= or $–CH_2–$

methylidyne HC≡

methylol (hydroxymethyl) $HOCH_2–$

(methylthio) MeS–

mono Numerical prefix denoting 'one'

monoterpenoids Terpenoids having a C_{10} skeleton. For a comprehensive treatment of monoterpenoids, see the *Dictionary of Natural Products*

morpholide An anion formed from morpholine by loss of the hydrogen attached to the nitrogen

morpholino 4-morpholinyl

multiplicative nomenclature A type of nomenclature used for some symmetrical molecules, which treats identical structural fragments only once in a name. In a multiplicative name, a 'multiplying radical' is used to express the presence of more than one occurrence of the preferred parent.

Multiplicative names are usually shorter and simpler than those that would be derived by normal substitutive nomenclature. For example: $HOOCCH_2SCH_2COOH$ is 2,2′-thiobisacetic acid (multiplicative name) rather than 2-[(carboxymethyl)thio]acetic acid (substitutive name).

Examples of multiplying radicals:

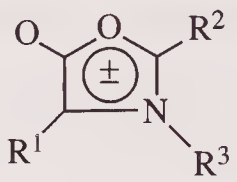
–O–	oxy
–NH–	imino
–N<	nitrilo
–S–	thio
–SS–	dithio
–S(O)–	sulfinyl
$–S(O)_2–$	sulfonyl
$–CH_2–$	methylene
$–CH_2CH_2–$	1,2-ethanediyl
–NMe–	(methylimino)

Although multiplicative names are not especially common, they are used in *Chemical Abstracts* for some well known compounds. For example:

EtOEt	1,1′-oxybisethane
MeS(O)Me	sulfinylbismethane
$HOCH_2CH_2NHCH_2CH_2OH$	2,2′-iminobisethanol

multiplicative prefixes See *numerical prefixes*

munchnones Mesoionic oxazolin-5-ones



munchnones

mustards $(SCH_2CHRX)_2$ X = halogen

mustard oils An old term for isothiocyanates

myristoyl (1-oxotetradecyl) $H_3C(CH_2)_{12}CO–$

myristyl tetradecyl $H_3C(CH_2)_{13}–$

n- Abbreviation for normal (unbranched) as in *n*-butane

N- 'nitrogen' used as a locant as in *N*-methylacetamide

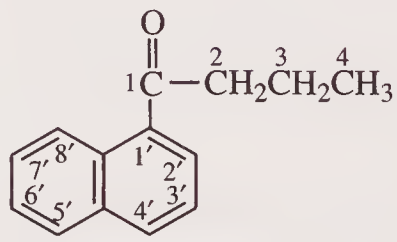
naphthenyl (naphthalenylmethylidyne) $(C_{10}H_7)C≡$

naphthionyl [(4-amino-1-naphthalenyl)sulfonyl] $4,1\text{-}H_2NC_{10}H_7SO_2–$

naphtho The ring fusion prefix derived from naphthalene

naphthobenzyl (naphthalenylmethyl) $(C_{10}H_7)CH_2–$

-naphthone Suffix denoting a ketone with formula $RCOC_{10}H_7$ ($C_{10}H_7$ = 1- or 2- naphthyl); '-onaphthone' replaces the '-ic acid' or '-oic acid' in the name of RCOOH



1′-butyronaphthone

naphthoxy (naphthalenyloxy) $(C_{10}H_7)O–$

naphthoyl (naphthalenylcarbonyl) $(C_{10}H_7)CO–$

naphthyl Contracted form of naphthalenyl

naphthylene naphthalenediyl

nazyl (naphthalenylmethyl) $(C_{10}H_7)CH_2–$

neo (Greek 'new') Used for a new stereoisomer (e.g. neomenthol); for hydrocarbons, a quaternary branched isomer (e.g. neopentane). In terpenes, the prefix 'neo' indicates the bond migration that

converts a *gem*-dimethyl grouping, directly attached to a ring carbon, into an isopropyl group. See the *Dictionary of Natural Products*

neopentyl (2,2-dimethylpropyl) $(H_3C)_3CCH_2$–

neophyl 2-methyl-2-phenylpropyl $PhC(CH_3)_2CH_2$–

neosteroids Occasionally used to refer to ring B aromatic steroids

nicotinoyl (3-pyridinylcarbonyl)

nitramino (nitroamino) O_2NNH–

nitrenes Neutral derivatives of monovalent nitrogen including the parent compound HN: (nitrene or imidogen)

nitrile oxides Compounds RC≡N(O). Thus, benzonitrile oxide is PhCNO

nitriles Compounds RCN. The suffix '-nitrile' denotes a –CN group at the end of an aliphatic chain. Thus, butanenitrile is $H_3CCH_2CH_2CN$. In DOC 6, most nitriles are entered as derivatives of the parent acids. Nitriles can also be named as cyano-substituted compounds, and this alternative is usually given in DOC 6

2-furannitrile or 2-cyanofuran

nitrilimine $HC≡N^+–N^-H$

nitrilio $HN^+≡$

nitrilo N≡

nitrimines (nitroimines) $RR'C=NNO_2$

nitro O_2N–'nitro compounds' are compounds RNO_2

***aci*-nitro** HON(O)=

nitrogen mustards $RN(CH_2CHRX)_2$ X = halogen

nitrolic acids Compounds $RC(=NOH)NO_2$

nitrones *N*-Oxides of imines. Compounds containing the grouping C=N(O)R

nitronic acids *aci*-Nitro compounds, $R^1R^2C=N(O)OH$

nitrosamino (nitrosoamino) ONNH–

nitrosimino (nitrosoimino) ONN=

nitroso ON– Nitroso compounds are compounds RNO

nitrosolic acids Compounds RC(=NOH)NO

nitroxides Free radicals derived from *N*-hydroxy amines by loss of the hydrogen from the oxygen atom, i.e. $R^1R^2N–O\cdot$. Thus, dimethyl nitroxide is $Me_2N–O\cdot$

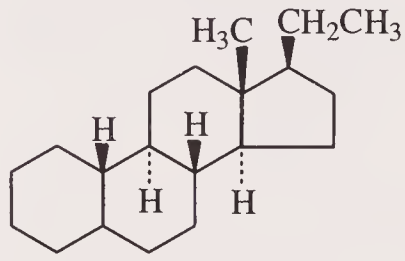
nona Numerical prefix denoting 'nine'. Nonaconta denotes '90', nonacosa denotes '29', and nonadeca denotes '19'

nonanoyl (1-oxononyl) $H_3C(CH_2)_7CO$–

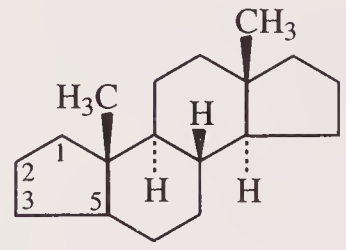
nonose An aldose with nine carbon atoms

nonulose A ketose with nine carbon atoms

nor Used mainly in naming steroids and terpenes, 'nor' denotes elimination of one CH_2 group from a chain or contraction of a ring by one CH_2 unit.



19-norpregnane



A-norandrostane

In older usage, particularly for monoterpenes, 'nor' denotes loss of all methyl groups attached to a ring system, e.g. norbornane, norpinane. The plural form should be *bisnor* when two carbon atoms are lost from the same site and *dinor* where they are lost from different sites, but in practice the terms are used interchangeably

norbornyl A contracted form of norbornanyl, the radical derived from norbornane

norcaryl A contracted form of norcaranyl, the radical derived from norcarane

norleucyl $H_3C(CH_2)_3CH(NH_2)CO$– The acyl radical from norleucine used in naming peptides. In this case the prefix 'nor' means normal, i.e. the straight-chain isomer of leucine

norpinyl A contracted form of norpinanyl, the radical derived from norpinane

norvalyl $H_3CCH_2CH_2CH(NH_2)CO$– The acyl radical from norvaline used in naming peptides

nosyl [(4-nitrophenyl)sulfonyl] $4\text{-}O_2NC_6H_4SO_2$–

novi Numerical prefix denoting 'nine'. Used only in ring assembly names

nucleoside bases The most common bases found in nucleosides, together with their three-letter abbreviations, are given in Table 8.9

nucleosides Hydrolytic products of nucleic acids. *N*-Glycosyl derivatives of heterocyclic bases, the most common of which are purine and pyrimidine derivatives. Abbreviations used for nucleosides are shown in Table 8.10

nucleotides Phosphorylated nucleosides

numerical prefixes The numerical prefixes shown

Table 8.9 Common nucleoside bases and their abbreviated forms[a]

Ade	adenine
Cyt	cytosine
Gua	guanine
Hyp	hypoxanthine
Oro	orotate
Pur	unknown purine
Pyr	unknown pyrimidine
Shy	thiohypoxanthine
Sur	thiouracil
Thy	thymine
Ura	uracil
Xan	xanthine

[a] See DOC 6 for the structures.

in Table 8.11 are the ones commonly used in chemical nomenclature. See *Pure Appl. Chem.*, 1986, **58**, 1693

The prefixes bis, tris, tetrakis, pentakis, hexakis, etc., are used with complex terms and to avoid ambiguity. The prefixes bi, ter, quater, quinque, sexi, etc., are used in naming ring assemblies (see *ring assemblies*)

Table 8.10 Abbreviations for nucleosides

Ado	A	adenosine
BrUrd	B	5-bromouridine
Cyd	C	cytidine
	D or hU	5,6-dihydrouridine
Guo	G	guanosine
Ino	I	inosine
Nuc	N	unspecified nucleoside
Oro	O	orotidine
Puo	R	unspecified purine nucleoside
Pyd	Y	unspecified pyrimidine nucleoside
ψrd	ψ or Q	pseudouridine
Sno	M or sI	thiouridine
Srd	S or sU	6-thioinosine
Thd	T	ribosylthymine (not thymidine)
Urd	U	uridine
Xao	X	xanthosine
d		2-deoxy
dThd	dT	thymidine
Nir		ribosylnicotinamide
-P		phosphoric residue

Table 8.11 Common numerical prefixes

1	mono	27	heptacosa
2	di	28	octacosa
3	tri	29	nonacosa
4	tetra	30	triaconta
5	penta	31	hentriaconta
6	hexa	32	dotriaconta
7	hepta	33	tritriaconta
8	octa	40	tetraconta
9	nona	50	pentaconta
10	deca	60	hexaconta
11	undeca	70	heptaconta
12	dodeca	80	octaconta
13	trideca	90	nonaconta
14	tetradeca	100	hecta
15	pentadeca	101	henhecta
16	hexadeca	102	dohecta
17	heptadeca	110	decahecta
18	octadeca	120	eicosahecta or icosahecta
19	nonadeca		
20	eicosa or icosa	130	triacontahecta
21	heneicosa or henicosa	200	dicta
		300	tricta
22	docosa	400	tetracta
23	tricosa	1000	kilia
24	tetracosa	2000	dilia
25	pentacosa	3000	trilia
26	hexacosa	4000	tetrilia

o- Abbreviated form of *ortho-*

O- 'Oxygen' used as a locant

-ocane, -ocin, -ocine Hantzsch–Widman stems for eight-membered heterocyclic rings. See *Hantzsch–Widman names*

octa Numerical prefix denoting 'eight'. Octaconta denotes '80', octacosa denotes '28', and octadeca denotes '18'

octadecanoyl (1-oxooctadecyl) $H_3C(CH_2)_{16}CO–$

octanoyl (1-oxooctyl) $H_3C(CH_2)_6CO–$

octi Numerical prefix denoting 'eight'. Used only in ring assembly names

octose An aldose with eight carbon atoms

octulose A ketose with eight carbon atoms

***tert*-octyl** (1,1,3,3-tetramethylbutyl) $(H_3C)_3CCH_2C(CH_3)_2–$

oenanthyl See *enanthoyl*

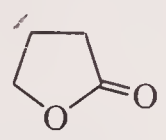
-oic acid Suffix denoting the –COOH group as part

of an aliphatic chain. Thus, butanoic acid is $H_3CCH_2CH_2COOH$

-oin Suffix denoting an acyloin RCH(OH)COR. The acyloin name is derived by changing the ending '-ic acid' or '-oic acid' in the name of RCOOH to '-oin'. Thus, benzoin is PhCH(OH)COPh

-ol Suffix denoting the --OH group in alcohols and phenols

-olactone Suffix denoting a lactone



γ-butyrolactone

-olane Hantzsch–Widman stem for a five-membered saturated heterocyclic ring not containing nitrogen

-olate Suffix denoting a salt of an alcohol. Thus, sodium methanolate is MeONa

-ole Hantzsch–Widman stem for a five-membered fully unsaturated heterocyclic ring

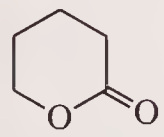
olefins Compounds containing one or more double bonds. 'Alkenes' is now the more usual term

-olene Hantzsch–Widman stem for a five-membered saturated heterocyclic ring containing one double bond but no nitrogen

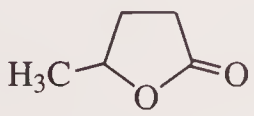
oleoyl (1-oxo-9-octadecenoyl) $H_3C(CH_2)_7CH{=}CH(CH_2)_7CO–$

oleyl (*Z*)-9-octadecenyl $H_3C(CH_2)_7CH{=}CH(CH_2)_8–$

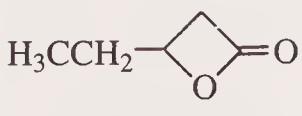
-olide Suffix denoting a lactone



5-pentanolide



4-pentanolide



3-pentanolide

-olidine Hantzsch–Widman stem for a five-membered saturated heterocyclic ring containing nitrogen

oligo Prefix meaning 'a few' as in oligosaccharides

-oline Hantzsch–Widman stem for a five-membered heterocyclic ring containing nitrogen and one double bond

-olium Denotes a positively charged species derived from a base with a name ending in -ole, e.g. pyrrolium

-onane Hantzsch–Widman stem for a nine-membered saturated heterocyclic ring not containing nitrogen

-onaphthone See *-naphthone*

-one Suffix denoting the presence of a ketone group

-onic acid See *aldonic acids*

-onin, -onine Hantzsch–Widman stems for nine-membered heterocyclic rings. See *Hantzsch–Widman names*

-onitrile Replacement of the '-ic acid' or '-oic acid' suffix of trivially named acids by '-onitrile' denotes replacement of –COOH by –CN. Thus, acetonitrile is H_3CCN

-onium Indicates a positively charged species such as ammonium, phosphonium, sulfonium, oxonium, etc.

-ophenone See *-phenone*

ornithyl $H_2N(CH_2)_3CH(NH_2)CO–$ The acyl radical from ornithine used in naming peptides

ortho- Denotes 1,2-substitution in a benzene ring (abbreviated to *o-*)

ortho- The highest-hydrated form of an acid, e.g. orthocarbonic acid, $C(OH)_4$

orthoesters Compounds $R^1C(OR^2)_3$, esters of the hypothetical ortho acids $R^1C(OH)_3$. Thus, ethyl orthoacetate is $H_3CC(OEt)_3$; orthoacetic acid is $H_3CC(OH)_3$

osazones Dihydrazones having the two hydrazone groups attached to adjacent carbon atoms. They are formed from compounds having the groupings –COCO– or –CH(OH)CO–, in the latter case with formal oxidation of the hydroxy group

-oside Suffix denoting a glycoside. See *glycoside*

-osyl Suffix denoting a glycosyl radical. See *glycosyl*

oxa Replacement prefix denoting an oxygen atom

oxalaceto (3-carboxy-1,3-dioxopropyl) $HOOCCOCH_2CO–$

oxalacetyl (1,2,4-trioxo-1,4-butanediyl) $–COCH_2COCO–$

oxalo (carboxycarbonyl) HOOCCO–

oxalyl (1,2-dioxo-1,2-ethanediyl) –COCO–

oxamoyl or **oxamyl** (aminooxoacetyl) $H_2NCOCO–$

oxides Ethers have sometimes been named as oxides. Compounds R^1OOR^2 are dioxides, R^1OOOR^3 are trioxides, etc. Thus, dimethyl oxide is Me_2O, dimethyl dioxide is MeOOMe, dimethyl trioxide is MeOOOMe, etc. Also, an alkene oxide is the epoxide derived from that alkene. Thus, styrene oxide is phenyloxirane. In addition, 'oxide' sometimes denotes the salt of an alcohol. Thus, sodium benzyloxide is $PhCH_2ONa$. Finally,

'oxide' is used to indicate addition of O= at a heteroatom as in trimethylamine *N*-oxide (Me_3NO), phosphine oxide ($H_3P{=}O$) and pyridine *N*-oxide

oxido Sometimes used to mean 'epoxy'. Also used as a substituent prefix to denote O= attached to a heteroatom as in amine oxides; thus, 1-oxidopyridine is pyridine *N*-oxide

oximes Compounds RCH=NOH or $R^1R^2C{=}NOH$ considered to derive from carbonyl compounds. Thus, acetaldehyde oxime is $H_3CCH{=}NOH$ and acetamide oxime is $H_3CC(=NOH)NH_2$

oximido (hydroxyimino) HON=

oxo O=

oxonia Replacement prefix denoting a positively charged oxygen atom

oxonio H_2O^+–

oxonium H_3O^+

oxy –O– Usually used when the free valencies are attached to different atoms that are not otherwise connected. Thus, 2,2′-oxydiethanol is $O(CH_2CH_2OH)_2$. 'Dioxy' is –OO–, 'trioxy' is –OOO-, etc.

-oyl Suffix denoting an acyl radical

ozonides 1,2,4-Trioxolanes formed by reaction of ozone at a C=C double bond

p- Abbreviation for *para-*

palmitoyl (1-oxohexadecyl) $H_3C(CH_2)_{14}CO$–

para- (Greek 'beside', 'beyond') denotes 1,4-substitution in a benzene ring

paracyclophanes Cyclophanes in which the benzene rings are *para*-substituted by the aliphatic bridging chains

paraffins Alkanes (obsol.)

pelargonoyl or **pelargonyl** (1-oxononyl) $H_3C(CH_2)_7CO$–

penta Numerical prefix denoting 'five'. Pentaconta denotes '50', pentacosa denotes '25', and pentadeca denotes '15'

pentadecanoyl (1-oxopentadecyl) $H_3C(CH_2)_{13}CO$–

pentakis Numerical prefix used instead of 'penta' with complex terms and to avoid ambiguity

pentamethylene 1,5-pentanediyl $-(CH_2)_5-$

pentitol An alditol with five carbon atoms

pentose An aldose with five carbon atoms

pentulose A ketose with five carbon atoms

pentyl $H_3C(CH_2)_4-$

***tert*-pentyl** (1,1-dimethylpropyl) $H_3CCH_2C(CH_3)_2-$

peptides Oligomers and polymers notionally derived from amino acids by condensation to produce amide linkages. For a list of amino acid abbreviations used in representing peptides, see *amino acids* (Table 8.1). Peptides are named either systematically or by trivial names. Trivial names of peptides can be modified in the following ways to denote a change in the amino acid sequence.

Replacement. When a peptide with a trivial name has an amino acid replaced by another amino acid, the modified peptide can be named as a derivative of the parent peptide by citing the new amino acid as a replacement. The new amino acid is designated by the appropriate amino acid residue number.

Extension. Extension of a trivially named peptide at the N-terminal end is denoted by substitutive nomenclature. Extension at the C-terminal end is made by citing the new amino acid residues with locants derived by suffixing the highest locant with a, b, etc. Extension in the middle of the chain is denoted by use of the term *endo-*.

Removal. Removal of an amino acid residue is denoted using 'de-'.

H-Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg-OH
1 2 3 4 5 6 7 8 9
bradykinin

H-Arg-Pro-Pro-Gly-Phe-Ser-Phe-Phe-Arg-OH
7-L-phenylalaninebradykinin

H-Lys-Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg-OH
N^2-L-lysylbradykinin

H-Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg-Arg-OH
9a-L-argininebradykinin

H-Arg-Pro-Pro-Gly-Phe-Ser-Ala-Pro-Phe-Arg-OH
6a-*endo*-L-alaninebradykinin

H-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg-OH
1-de-L-argininebradykinin

For further information on the nomenclature and symbolism of peptides, See *Pure Appl. Chem.*, 1984, **56**, 595

per The highest state of oxidation, e.g. perchloric acid. Presence of a peroxide (–O–O–) group, e.g. perbenzoic acid. Also, exhaustive substitution or addition, e.g. perhydronaphthalene (= decahydronaphthalene)

perchloro Denotes that all hydrogen atoms (except those which are part of functional groups, e.g. CHO, COOH) have been replaced by chlorine atoms

perchloryl $O_3Cl–$

perfluoro Denotes that all hydrogen atoms (except those which are part of functional groups, e.g. CHO, COOH) have been replaced by fluorine atoms

perhydro Denotes full hydrogenation of a fused polycyclic system

peri The 1,8-substitution pattern in naphthalene (obsol.). Also, fusion of a ring to two or more adjoining rings, e.g. perinaphthindene

peroxides Compounds $R^1O–OR^2$. Thus, ethyl phenyl peroxide is EtOOPh and dibenzoyl peroxide is BzOOBz

-peroxoic acid Suffix denoting –C(O)OOH as part of an aliphatic chain. Thus, propaneperoxoic acid is $H_3CCH_2C(O)OOH$

peroxy acids Acids containing the group –C(O)OOH. Thus, peroxypropanoic acid is $H_3CCH_2C(O)OOH$ (also named as propane-peroxoic acid)

perylo The ring fusion prefix derived from perylene

phenacyl (2-oxo-2-phenylethyl) $PhCOCH_2–$

phenacylidene (2-oxo-2-phenylethylidene) PhCOCH=

phenanthro The ring fusion prefix derived from phenanthrene

phenanthryl Contracted form of phenanthrenyl

phenanthrylene phenanthrenediyl

phenenyl benzenetriyl '*as*-Phenenyl' is 1,2,4-benzenetriyl, '*s*-phenenyl' is 1,3,5-benzenetriyl, and '*vic*-phenenyl' is 1,2,3-benzenetriyl

phenethyl (2-phenylethyl) $PhCH_2CH_2–$

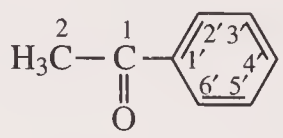
phenethylidene (2-phenylethylidene) $PhCH_2CH=$

phenetidides *N*-(Ethoxyphenyl) amides. They may be named analogously to anilides. Thus, aceto-*p*-phenetidide is *N*-(4-ethoxyphenyl)acetamide $H_3CCONHC_6H_4OEt$-4 (obsol.)

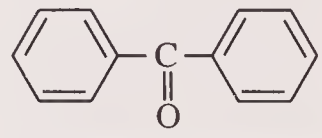
pheniodide, phenobromide, phenochloride Indicates a base that has been (formally) quaternised with phenyl iodide, phenyl bromide or phenyl chloride (reaction not usually feasible in practice)

phenols Hydroxy derivatives of benzene and other aromatic carbocyclic systems

-phenone Suffix denoting a ketone with formula RCOPh; '-ophenone' replaces the '-ic acid' or '-oic acid' in the name of RCOOH



acetophenone



benzophenone

phenoxide The anion $PhO^–$. Thus, potassium phenoxide is PhOK

phenoxy PhO–

phenyl $C_6H_5–$ The radical from benzene. Often (invariably in DOC 6) denoted by Ph in structural formulae

phenylalanyl $PhCH_2CH(NH_2)CO–$ The acyl radical from phenylalanine, used in naming peptides

phenylene $–(C_6H_4)–$ Also called 'benzenediyl'. Thus, *o*-phenylene or 1,2-phenylene is 1,2-benzenediyl

phospha Replacement prefix denoting a phosphorus atom

phosphatidic acids Derivatives of glycerol in which one primary OH group is esterified with phosphoric acid and the other two OH groups are esterified with fatty acids

phosphazines Compounds containing the group =C=N–N=P≡, e.g. $(H_3C)_2C=N–N=PPh_3$

phosphazo –P=N–

phosphenic acid $(HO)PO_2$

phosphenous acid (HO)PO

phosphine PH_3 'Phosphine imine' is $H_3P=NH$, 'phosphine oxide' is $H_3P=O$ anphosphine sulfide' is $H_3P=S$. 'Diphosphine' is H_2PPH_2, 'triphosphine' is H_2PPHPH_2, etc.

phosphinic acid $(HO)H_2PO$

phosphinico HOP(O)= (multiplying radical)

phosphinidene HP=

phosphinidyne P≡

phospinimyl $H_2P(=NH)–$

phosphino $H_2P–$

phosphinothioyl $H_2P(S)–$

phosphinous acid $(HO)H_2P$

phosphinoyl $H_2P(O)–$ (IUPAC)

phosphinyl $H_2P(O)–$ (CAS)

phosphinylidene HP(O)=

phosphinylidyne P(O)≡

phosphite Denotes a salt or ester of phosphorous acid

phospho O_2P– 'Phospho' is occasionally used in place of phosphono to denote the group –P(O)$(OH)_2$ when attached to atoms other than C, e.g. as in phosphocholine, $Me_3N^+CH_2CH_2OP(O)(OH)(O^-)$

phosphonic acid $(HO)_2HP(O)$

phosphonio H_3P^+–

phosphonitridyl $H_2P(\equiv N)$–

phosphonium H_4P^+

phosphono $(HO)_2P(O)$–

phosphonous acid $(HO)_2HP$

phosphonoyl phosphinylidene HP(O)=

phosphorane PH_5

phosphoranyl H_4P–

phosphoranylidene H_3P=

phosphoranylidyne $H_2P\equiv$

phosphoric acid $(HO)_3PO$ 'Diphosphoric acid' is $(HO)_2P(O)OP(O)(OH)_2$, 'triphosphoric acid' is $(HO)_2P(O)OP(O)(OH)OP(O)(OH)_2$, etc.

phosphoro 1,2-diphosphenediyl –P=P–

phosphorodithioic acid $(HO)_2P(S)SH$ or $(HO)P(O)(SH)_2$

phosphoroso OP–

phosphorothioic acid $(HO)_3P(S)$ or $(HO)_2P(O)(SH)$

phosphorous acid $(HO)_3P$

phosphorus compounds Many phosphorus (and arsenic) compounds are named using functional replacement nomenclature in which replacement affixes are inserted into the names of the appropriate phosphorus (arsenic) acids (Table 8.12). For full coverage of organoarsenic compounds see the *Dictionary of Organometallic Compounds.*

Acidic functional replacement analogues of mononuclear phosphorus and arsenic acids are named by citing the functional replacement affixes in alphabetical order just preceding the '-ic acid' or '-ous acid'. The affixes used are listed in Table 8.13.

Table 8.13 Functional replacement affixes for phosphorus and arsenic compounds

Affix	Replacement operation
amido	–OH by $–NH_2$
azido	–OH by $–N_3$
bromido	–OH by –Br
chlorido	–OH by –Cl
cyanatido	–OH by –OCN
cyanido	–OH by –CN
(dithioperoxo)	–OH by –SSH
fluorido	–OH by –F
hydrazido	–OH by $–NHNH_2$
imido	=O by =NH
iodido	–OH by –I
isocyanitido	–OH by –NCO
(isothiocyanitido)	–OH by –NCS
nitrido	=O and –OH by ≡N
peroxo	–OH by –OOH
seleno	=O by =Se or –OH by –SeH
telluro	=O by =Te or –OH by –TeH
thio	=O by =S or –OH by –SH
(thiocyanitido)	–OH by –SCN

Table 8.12 Parent acid names used in functional replacement nomenclature of phosphorus and arsenic compounds

Trivalent acids			
$(HO)_3P$	phosphorous acid	$(HO)_3As$	arsenous acid
$(HO)_2HP$	phosphonous acid	$(HO)_2HAs$	arsonous acid
$(HO)H_2P$	phosphinous acid	$(HO)H_2As$	arsinous acid
(HO)PO	phosphenous acid	(HO)AsO	arsenenous acid
Pentavalent acids			
$(HO)_3PO$	phosphoric acid	$(HO)_3AsO$	arsenic acid
$(HO)_2HPO$	phosphonic acid	$(HO)_3HAsO$	arsonic acid
$(HO)H_2PO$	phosphinic acid	$(HO)H_2AsO$	arsinic acid
$(HO)PO_2$	phosphenic acid	$(HO)AsO_2$	arsenenic acid

The following examples are derived from phosphoric acid:

$(H_2N)(HO)_2PO$	phosphoramidic acid
$Br(HO)_2PO$	phosphorobromidic acid
$Cl_2(HO)PO$	phosphorodichloridic acid
$(HS)_3P{=}NH$	phosphorimidotrithioic acid

Non-acidic functional replacement analogues are named by replacing the word 'acid' by the appropriate class name occurring earliest in the following list: hydrazide, halide, azide, amide, cyanide, isocyanide, cyanate, thiocyanate, isothiocyanate, nitride, imide. Other replacing groups are denoted by infixes as described earlier for acidic functional replacement analogues. The following examples are derived from phosphoric acid:

$(H_2N)_3PO$	phosphoric triamide
$Cl_3P{=}NH$	phosphorimidic trichloride
$(H_2N)_2(N_3)PO$	phosphorodiamidic azide

phosphoryl phosphinylidyne P(O)≡

phthalimido (1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)

phthaloyl (1,2-phenylenedicarbonyl) $1,2\text{-}C_6H_4(CO–)_2$

phthalyl (2-carboxybenzoyl) $2\text{-}HOOCC_6H_4CO–$

picolinoyl (2-pyridinylcarbonyl)

picrate Denotes an ester, salt or addition compound of picric acid

picryl (2,4,6-trinitrophenyl) $2,4,6\text{-}(O_2N)_3C_6H_2–$

pimeloyl (1,7-dioxo-1,7-heptanediyl) $–CO(CH_2)_5CO–$

pinacols A general term for tetrasubstituted 1,2-ethanediols. 'Pinacol' is 2,3-dimethyl-2,3-butanediol $(H_3C)_2C(OH)C(OH)(CH_3)_2$

pipecoloyl (2-piperidinylcarbonyl)

piperidide An anion formed from piperidine by loss of the hydrogen attached to the nitrogen

piperidino 1-piperidinyl

piperidyl A contracted form of piperidinyl

piperonyl 1,3-benzodioxol-5-ylmethyl (= 3,4-methylenedioxybenzyl)

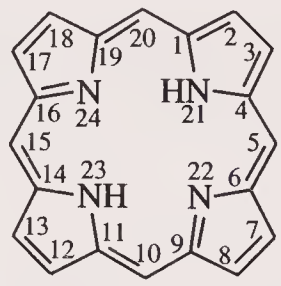
pipsyl [(4-iodophenyl)sulfonyl)] $4\text{-}IC_6H_4SO_2–$

pivaloyl or **pivalyl** (2,2-dimethyl-1-oxopropyl) $(H_3C)_3CCO–$

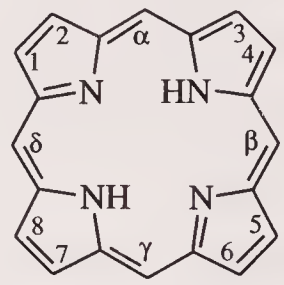
poly Many

polypyrroles See *tetrapyrroles*

porphyrins Cyclic tetrapyrrolic structures in which each of the four pyrrole rings is linked to two others by single methylidyne groups. The parent system is called porphyrin (IUPAC) or porphine (CAS). In the old literature, the so-called Fischer numbering may be encountered.



21*H*,23*H*-porphine or porphyrin



Fischer numbering

For a comprehensive treatment of naturally occurring porphyrins, see the *Dictionary of Natural Products*

prenyl (3-methyl-2-butenyl) $(H_3C)_2C{=}HCHCH_2–$ Also called isoprenyl or γ,γ–dimethylallyl

prolyl (2-pyrrolidinylcarbonyl) The acyl radical from proline used in naming peptides

propargyl 2-propynyl $HC{\equiv}CCH_2–$

propioloyl or **propiolyl** (1-oxo-2-propynyl) $HC{\equiv}CCO–$

propionyl (1-oxopropyl) $H_3CCH_2CO–$

propoxy $H_3CCH_2CH_2O–$

propyl or ***n*-propyl** $H_3CCH_2CH_2–$ Often abbreviated to Pr (or Pr^n or *n*-Pr) in structural and line formulae

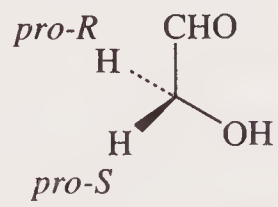
***sec*-propyl** (1-methylethyl) $(H_3C)_2CH–$ (obsol.)

propylene (radical) (1-methyl-1,2-ethanediyl) $–CH(CH_3)CH_2–$

propylidene $H_3CCH_2CH{=}$

propylidyne $H_3CCH_2C{\equiv}$

pro-R, pro-S These terms are used to distinguish an identical pair of atoms or groups in a prochiral compound. That one which leads to an (*R*)-compound when considered to be preferred to the other by the sequence rule (without changing the priority with respect to the other substituents) is termed *pro-R*; the other is termed *pro-S*



proteins Polypeptides of high molecular weight (above about 10 000). See *amino acids* (Table 8.1) for a list of amino acid abbreviations used in denoting proteins.

protocatechuoyl (3,4-dihydroxybenzoyl) $3,4\text{-}(HO)_2C_6H_3CO–$

pseudo (Greek 'false') Prefix indicating resemblance to, especially isomerism with, e.g. pseudocumene or ψ-cumene. DOC 6 indexes both versions

pseudoallyl (1-methylethenyl) $H_2C{=}C(CH_3)–$

pseudocumyl (trimethylphenyl) '*as*-Pseudocumyl' is (2,3,5-trimethylphenyl), '*s*-pseudocumyl' is (2,4,5-trimethylphenyl) and '*v*-pseudocumyl' is (2,3,6-trimethylphenyl) (obsol.)

pyranoses Cyclic hemiacetal forms of monosaccharides in which the ring is six-membered. See *carbohydrates*

-pyranoside Denotes a glycoside containing a pyranose ring. See *glycoside*

-pyranosyl Denotes a radical formed from a pyranose form of a monosaccharide by detaching the anomeric OH group

pyrido The ring fusion prefix derived from pyridine

pyridyl Contracted form of pyridinyl

pyrimido The ring fusion prefix derived from pyrimidine

pyrimidyl A contracted form of pyrimidinyl

pyroglutamyl (5-oxoprolyl)

pyromucyl (2-furanylcarbonyl)

pyrophosphoric acid Diphosphoric acid, $(HO)_2P(O)OP(O)(OH)_2$

pyrophosphorous acid Diphosphorous acid, $(HO)_2POP(OH)_2$

pyrromethenes Compounds containing two pyrrole rings joined by a –CH= group

pyrroyl (pyrrolylcarbonyl)

pyrryl Contracted form of pyrrolyl

pyruvoyl (1,2-dioxopropyl) $H_3CCOCO–$

quater Numerical prefix denoting 'four', used only in naming ring assemblies

quercitols Deoxyinositols, i.e. 1,2,3,4,5-cyclohexanepentols

quinaldoyl (2-quinolinylcarbonyl)

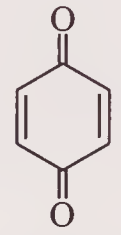
quino The ring fusion prefix derived from quinoline

quinomethides See *quinone methides*

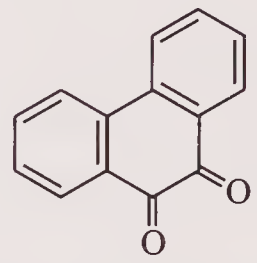
quinone imines or **quinonimines** Compounds derived from quinones by replacement of one or more of the quinone oxygens by HN=

quinone methides or **quinomethides** Compounds derived from quinones by replacement of one or more of the quinone oxygens by $H_2C{=}$

quinones Diketones derived from aromatic compounds by conversion of two CH groups into CO groups



p-benzoquinone



9,10-phenanthrenequinone or phenanthraquinone

quinonimines See *quinone imines*

quinonyl Denotes a radical formed by loss of hydrogen from a quinone, e.g. 1,4-benzoquinonyl

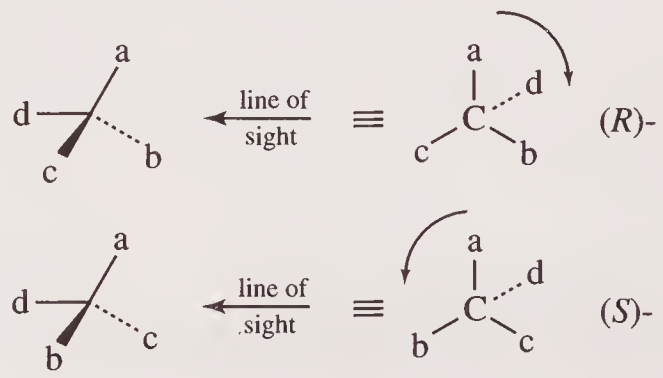
quinque Numerical prefix denoting 'five', used only in naming ring assemblies

r- Denotes the absolute configuration of a pseudo-asymmetric centre (variant of *R*-below)

R- An absolute stereochemical descriptor. The *R*- and *S*-system provides an unambiguous method of defining configuration about a chiral tetrahedral atom. The order of priority of the groups or atoms surrounding the tetrahedral atom is assigned using the sequence rule (*q.v.*) and *R*- and *S*- are then assigned as follows.

The molecule is viewed from opposite the group of lowest (fourth) priority. If the remaining groups in decreasing order of priority are arranged in a clockwise manner, then the configuration is *R*. If they are arranged in an anticlockwise manner, then the configuration is *S*.

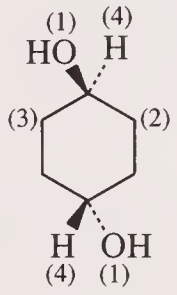
In the following diagrams the order of priority of the groups is a > b > c > d. Hence the molecule is viewed from opposite group d.

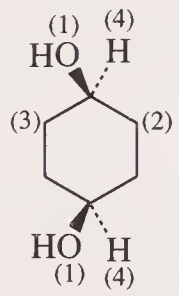


R_a and R_p are used to denote axial and planar chirality respectively.

***R**-** *R**- and *S**- are relative stereochemical descriptors. Thus, (*R**, *R**) indicates two centres of like chirality (either both *R*- or both *S*-) and (*R**, *S**) indicates two centres of unlike chirality. (*RS*) and (*SR*) are used to denote racemates (see *RS*-)

Note that (*R,S*)-descriptors can also be assigned to prochiral centres in more symmetrical molecules by a simple extension of the sequence rule. For example, in 1,4-cyclohexanediol the OH group at each centre has priority 1 and the H atom priority 4.





An *arbitrary* choice is made between the methylene chains (2) and (3), giving (1*RS*,4*RS*) chirality to the *trans* form and (1*RS*,4*SR*) to the *cis*. The result is independent of the arbitrary choice made.

***rac*-** Used with natural product names to denote a racemate. In a peptide name *rac*- denotes that all the amino acids are DL. The abbreviation *racem*- is found in *Beilstein*

radicofunctional nomenclature A radicofunctional name is one in which the principal function of the substance is expressed as a single-name term, while the remainder of the structure attached to this function is described by radicals. Examples of radicofunctional names are:

methyl alcohol	MeOH
ethyl methyl ketone	EtCOMe
dimethyl peroxide	MeOOMe

***rel*-** Denotes that the given configurations are relative and not absolute

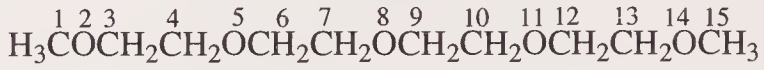
replacement nomenclature Organic replacement names are formed by denoting heteroatoms that replace skeletal atoms of a hydrocarbon molecular skeleton by organic replacement prefixes (Table 8.14). The prefixes are cited in the order they are given in the table. The prefix 'azonia' denotes replacement of a carbon atom by a positively charged nitrogen atom. Other prefixes for positively charged atoms are formed similarly, e.g. oxonia, thionia.

Table 8.14 Organic replacement prefixes

fluorine	fluora
chlorine	chlora
bromine	broma
iodine	ioda
astatine	astata
oxygen	oxa
sulfur	thia
selenium	selena
tellurium	tellura
nitrogen	aza
phosphorus	phospha
arsenic	arsa
antimony	stiba
bismuth	bisma
silicon	sila
germanium	germa
tin	stanna
lead	plumba
boron	bora

Elision of vowels is *not* practised in replacement nomenclature. Thus pentaoxa-not pentoxa-.

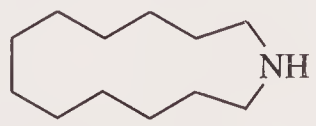
Replacement names can be used for chains of atoms, usually when there are four or more heteroatoms. It is especially useful for naming polyethers.



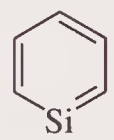
2,5,8,11,14-pentaoxapentadecane

4-oxa-2,6,8-triazanonan-1-ol

Replacement nomenclature is used for some heterocyclic systems, including von Baeyer systems, large rings (>10 members) and some spiro compounds.



azacyclotridecane



silabenzene

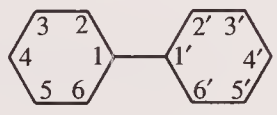
***retro*-** (in carotene names) The prefix *retro*- and a pair of locants denotes a shift, by one position, of all single and double bonds delineated by the pair of locants. The first locant cited is that of the carbon atom that has lost a proton, the second that of the carbon atom that has gained a proton

retro- (in peptide names) When used with a trivially named peptide, *retro-* denotes that the amino acid sequence is the reverse of that in the naturally occurring compound

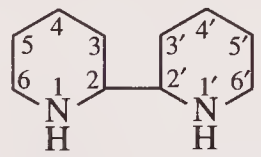
ribo- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

ring assemblies Ring assemblies are polycyclic systems consisting of two or more identical rings or ring systems directly joined to each other by single or double bonds. Linear assemblies joined by single bonds are named by citing a numerical prefix (Table 8.15) to the name of the ring or ring system (except for benzene and the cycloalkanes, when the appropriate radical name is used).

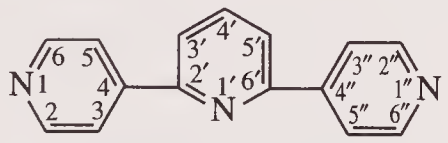
The numbering of the assembly is that of the component system. One terminal component is assigned unprimed numbers as locants, the locants of the other components being primed serially.



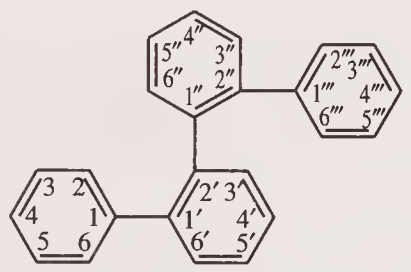
1,1′-bicyclohexyl



2,2′-bipiperidine

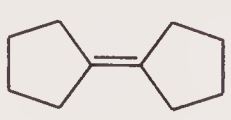


4,2′:6′,4″-terpyridine

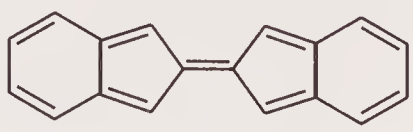


1,1′:2′,1″:2″,1‴-quaterphenyl
or *o*-quaterphenyl

Ring assembly names are sometimes applied to ring systems joined by a double bond



1,1′-bicyclopentylidene



$\Delta^{2,2'}$-bi-2*H*-indene

ring fusion names Examples of ring fusion names are:

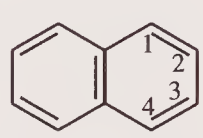
- Naphtho[2,3-*b*]furan
- Benzo[a]cyclopent[*j*]anthracene
- Dibenzo[*de,rst*]pentaphene
- Pyrido[1′,2′ :1,2]imidazo[4,5-*b*]quinoxaline

Table 8.15 Prefixes used in naming ring assemblies

No. of components	Numerical prefix
2	bi
3	ter
4	quater
5	quinque
6	sexi
7	septi
8	octi
9	novi
10	deci
11	undeci
12	dodeci
13	trideci
	etc.

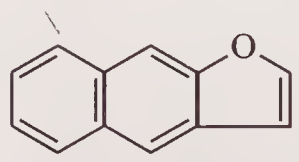
These names are derived by prefixing to the name of a component ring or ring system (the base component), designations of the other components. The prefixes are normally obtained by changing the ending '-e' of the name of the ring or ring system to '-o'; there are exceptions such as 'benzo', 'pyrido' and 'cyclopenta'. Isomers are distinguished by lettering the peripheral sides of the base component *a, b, c,* etc., beginning with *a* for side 1–2. To the letter denoting where fusion occurs are prefixed, if necessary, the numbers of the positions of attachment of the other component. The resulting name denotes the ring system containing the maximum number of non-cumulative double bonds. In cases where the parent ring system is unsystematically numbered, e.g. anthracene, the fusion lettering uses the 1,2-face as *a*, then proceeds round the ring sequentially regardless of the unsystematic numbering.

- Naphtho[2,3-*b*]furan



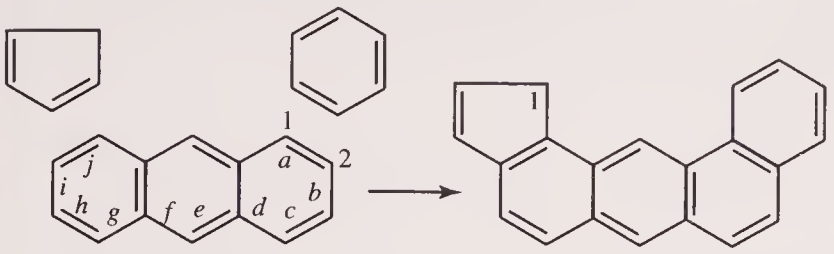
naphthalene
(fusion prefix = naphtho)

furan
(base component)



naphtho[2,3-*b*]furan

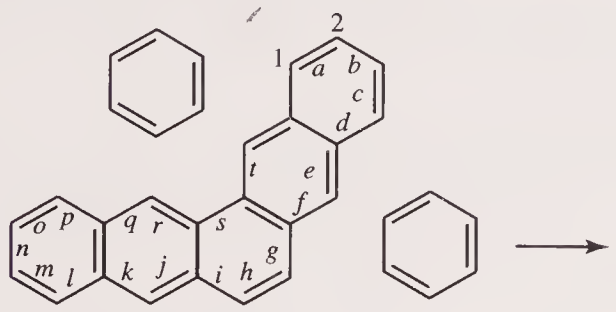
- Benzo[*a*]cyclopent[*j*]anthracene



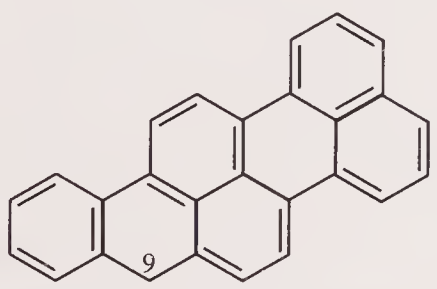
anthracene (base component)

1*H*-benzo[*a*]cyclopent[*j*]anthracene

- Dibenzo[*de,rst*]pentaphene

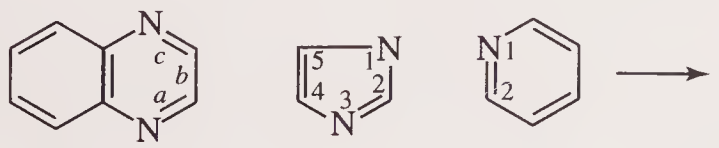


pentaphene (base component)



9*H*-dibenzo[*de,rst*]pentaphene

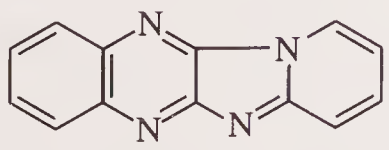
- Pyrido[1′,2′ : 1,2]imidazo[4,5-*b*]quinoxaline



quinoxaline (base component)

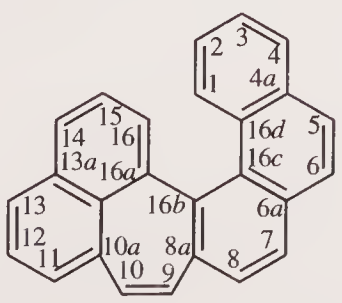
imidazo

pyrido



pyrido[1′,2′:1,2]imidazo[4,5-*b*]quinoxaline

Numbering of polycyclic systems. The system is oriented in such a way that gives (a) the greatest number of rings in a horizontal row and (b) a maximum number of rings above and to the right of the horizontal row. The system is then numbered in a clockwise direction commencing with the carbon atom not involved in ring fusion in the most anticlockwise position of the uppermost ring farthest to the right, Carbon atoms common to two or more rings are designated by adding roman letters 'a', 'b', 'c', etc., to the number of the position immediately preceding.



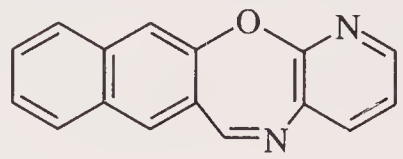
Ambiguities are resolved by assigning lowest possible numbers to (a) heteroatoms, (b) ring junctions and (c) indicated hydrogen

ring systems For various types of ring system, see *bridged ring systems Hantzsch–Widman names, ring assemblies, ring fusion names, spiro compounds* and *von Baeyer nomenclature.*

Various publications from Chemical Abstracts Service can be used to find the name of a known ring system. The most comprehensive source of ring system names is the *Ring Systems Handbook* (RSH) (successor to the *Parent Compound Handbook*). This was last issued in 1993 and cumulative supplements are issued every six months. Entries are in ring analysis order, i.e. it is arranged according to the following hierarcy of ring data:

1. Number of component rings.
2. Sizes of component rings.
3. Elemental analysis of component rings.

For example, the ring system:

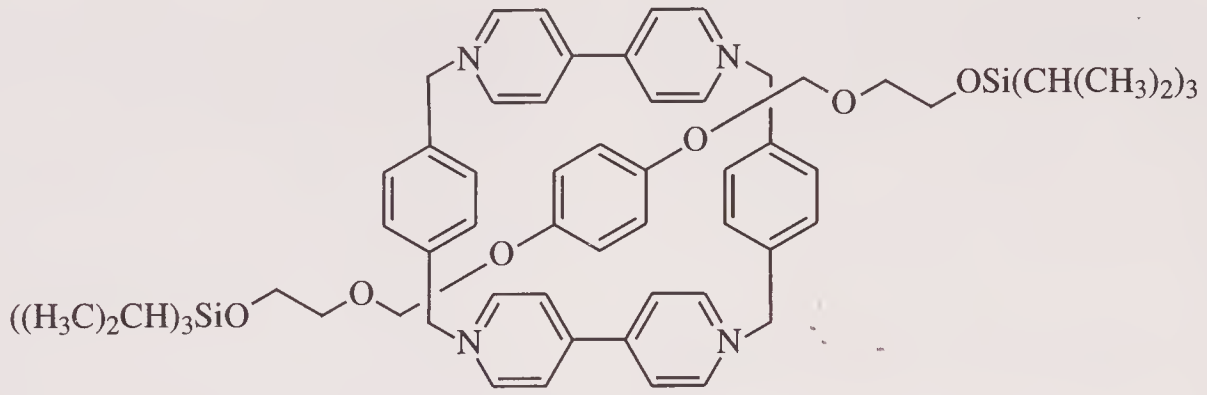


contains four rings; with sizes 6, 6, 6, 7; and with elemental compositions C_5N–C_6–C_6–C_5NO.

The *Ring Systems Handbook* also contains indexes of molecular formulae and CA Index Names. An 'Index of Ring Systems' can be found in each *Chemical Abstracts* Molecular Formula Index and gives all the ring systems indexed in that particular index. The *Chemical Abstracts* Index Guide for the 8th Collective Period (1967–71) contains an 'Index of Ring Systems' giving all ring systems known at that time.

rotaxanes A class of molecule in which an annular component is free to rotate around a spine, but is prevented from escape by end-groups on the spine. A prefix indicates the number of molecular components.

Stoddart, J. F., *et al., J. Am. Chem. Soc.,* 1992, **114,** 193



[2]rotaxane

RS- (*RS*)- and (*SR*)- are used to denote racemates of compounds with more than one chiral centre. Thus (1*RS*,2*SR*)- denotes a racemate compound consisting of the (1*R*,2*S*)- and (1*S*,2*R*)-enantiomers

s- Abbreviation for *symmetric(al)* as in *s*-triazine (1,3,5-triazine) and for *secondary* as in *s*-butyl

s- Stereochemical descriptor for a pseudosymmetric centre (variant of *S*- below)

S- An absolute stereochemical descriptor; see *R*. *S* also denotes sulfur as a locant

S*- A relative stereochemical descriptor. See *R**-

salicyl [(2-hydroxyphenylmethyl] 2-$HOC_6H_4CH_2$–

salicylidene [(2-hydroxyphenyl)methylene] 2-HOC_6H_4CH=

salicyloyl (2-hydroxybenzoyl) 2-HOC_6H_4CO–

sarcosyl (*N*-methylglycyl) $MeNHCH_2CO$–

Schardinger dextrins Another name for cyclodextrins

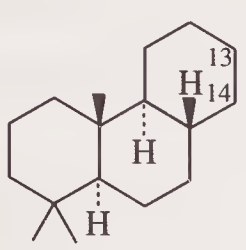
Schiff('s) bases See *azomethines*

sebacoyl (1,10-dioxo-1,10-decanediyl) $–CO(CH_2)_8CO–$

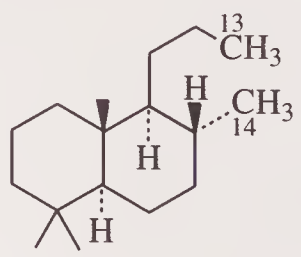
sec Abbreviation of *secondary* as in *sec*-butyl

***sec*-butyl** (1-methylpropyl) $H_3CCH_2CH(CH_3)–$

seco In steroid and terpene names, 'seco' denotes fission of a ring with addition of a hydrogen atom at each terminal group thus created



podocarpane



13,14-secopodocarpane

selena Replacement prefix denoting a selenium atom

-selenal Suffix denoting –C(Se)H when part of an aliphatic chain. Selenals are selenium analogues of aldehydes

-selenamide Suffix denoting $–SeNH_2$

-selenenic acid Suffix denoting –SeOH. Selenenic acids are selenium analogues of sulfenic acids

selenenimine $H_2Se=NH$

seleneno HOSe–

selenides Compounds R^1SeR^2, selenium analogues of ethers and sulfides. Compounds R^1SeSeR^2 are 'diselenides', $R^1SeSeSeR^2$ are 'triselenides', etc.

selenienyl The radical formed from selenophene by loss of a hydrogen

-seleninamide Suffix denoting $–Se(O)NH_2$

-seleninic acid Suffix denoting –Se(O)OH. Seleninic acids are selenium analogues of sulfinic acids

selenino HOSe(O)–

seleninyl OSe=

seleno Denotes replacement of oxygen by selenium as in selenourea, $(H_2N)_2C=Se$. Also denotes the bridging radical –Se–. Usually used when the free valencies are attached to different atoms that are not otherwise connected

selenocyanates Compounds RSeCN. Thus, methyl selenocyanate is MeSeCN

selenocyanato NCSe–

-selenol Suffix denoting –SeH. Selenols are selenium analogues of alcohols and thiols

-selenonamide Suffix denoting $–Se(O)_2NH_2$

selenones Compounds $R^1Se(O)_2R^2$, selenium analogues of sulfones. Thus, dimethyl selenone is $Me_2Se(O)_2$

-selenonic acid Suffix denoting $–Se(O)_2OH$. Selenonic acids are selenium analogues of sulfonic acids

selenonio $H_2Se^+–$

selenonium HSe^+

selenono $(HO)Se(O)_2–$

selenonyl $O_2Se–$

selenoxides Compounds $R^1Se(O)R^2$, selenium analogues of sulfoxides. Thus, dimethyl selenoxide is $Me_2Se(O)$

selenoxo Se= Usually used when both free valencies are attached to the same atom

selenyl HSe–

selones Compounds $R^1C(=Se)R^2$. Selenium analogues of ketones and thiones. Thus, 2-butaneselone is $H_3CC(=Se)CH_2CH_3$

semicarbazido [2-(aminocarbonyl)hydrazino] $H_2NCONHNH–$

semicarbazones Compounds $R^1R^2C=NNHCONH_2$. For example, acetone semicarbazone is $(H_3C)_2C=NNHCONH_2$

semioxamazones Compounds $R^1R^2C=NNHCOCONH_2$

senecioyl (3-methyl-1-oxo-2-butenyl) $(H_3C)_2C=CHCO–$

separable prefix A prefix to a chemical name that is detached and often inverted during indexing, e.g. *cis*- in *cis*-2-butene, which is indexed under 'B', either as '2-Butene, *cis*-' or (as in DOC 6) as '*cis*-2-Butene', with the italicised prefix being ignored at the first level by the indexing program. Descriptors such as *iso*- in *iso*-propyl were treated as separable in the old literature, but this is now obsolete. However, *tert*-butyl is still used

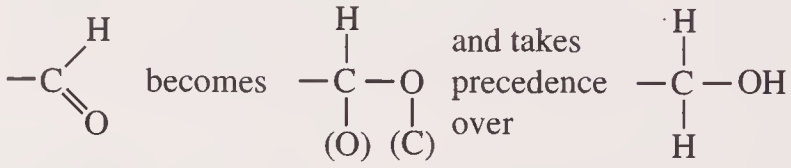
septanoses Cyclic hemiacetal forms of monosaccharides in which the ring is seven-membered

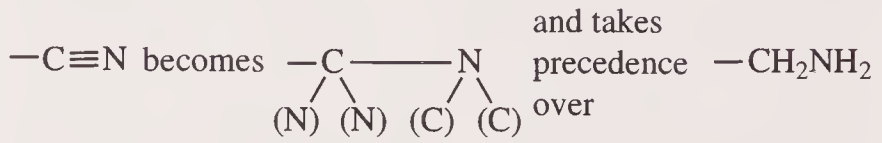
septi Numerical prefix denoting 'seven', used only in naming ring assemblies

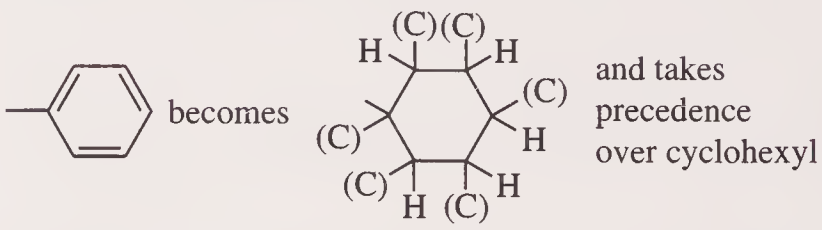
seqcis-, seqtrans- Equivalent to (*Z*)- and (*E*)-, respectively (obsol.)

sequence rule The sequence rule provides a method of arranging atoms or groups in an order of precedence. It is used in the assignment of stereochemical descriptors, for example, (*R*)-, (*S*)-, (*E*)- and (*Z*)-. The rules may be summarised as follows:

1. Atoms of higher atomic number take precedence over those of lower atomic number. Thus, $Cl > S > O > N > C > H$. Lone pairs are assigned the lowest possible priority.
2. Isotopes of higher atomic weight take precedence over those of lower atomic weight. Thus $^3H > ^2H > ^1H$.
3. When the first atoms in each group are the same, then the priorities are determined by the atomic numbers of the atoms that are directly attached to these. Thus $CH_2Cl > CH_2OH > CH_3$ because $Cl > O > H$ and $(H_3C)_3C > (H_3C)_2CH > H_3CCH_2$ because $C > H$. If no difference is observed for this second set of atoms, then the third set and the fourth and so on are considered in turn until there is a difference.
4. In groups containing a double or triple bond then, for the purposes of determining priority, the multiple bond is split into two or three bonds, as follows:







Only the multiply bonded atoms themselves are duplicated and not the atoms or groups attached to them.

5. When the difference between substituents is in configuration, then $Z > E$ and $R > S$.

Extensions of the sequence rule cover more complex examples of molecular chirality. Details can be found in the following articles:

Cahn, R. S., *et al., Angew. Chem., Int. Ed. Engl.,* 1966, **5**, 385

Cahn. R. S., *J. Chem. Educ.,* 1964, **41**, 116

IUPAC, *Nomenclature of Organic Chemistry*, p. 473

Prelog, V. *et al., Angew. Chem., Int. Ed. Engl.,* 1982, **21**, 567.

seryl $HOCH_2CH(NH_2)CO–$ The acyl radical from serine. Used in naming peptides

sesqui Numerical prefix meaning 1.5 as in sesquiterpenes and sesquihydrate

sesquiterpenoids Terpenoids having a C_{15} skeleton. Entries for a limited selection of the most important sesquiterpenoids are given in DOC 6. For a comprehensive treatment see the *Dictionary of Natural Products*

sester Numerical prefix meaning 2.5 as in sesterterpenes

sesterterpenes Terpenes having a C_{25} skeleton. For a comprehensive treatment see the *Dictonary of Natural Products*

sexi- Numerical prefix denoting 'six', used only in naming ring assemblies

siamyl (1,2-dimethylpropyl) $(H_3C)_2CHCH(CH_3)$–

sila Replacement prefix denoting a silicon atom

silane SiH_4 'Disilane' is H_3SiSiH_3, 'trisilane' is $H_3SiSiH_2SiH_3$, etc.

silanetetrayl =Si=

silathianes Compounds of general formula $H_3Si[SSiH_2]_nSSiH_3$, named 'disilathiane' (n = 0), 'trisilathiane' (n = 1), etc.

silazanes Compounds of general formula $H_3Si[NHSiH_2]_nNHSiH_3$, named 'disilazane' (n = 0), 'trisilazane' (n = 1), etc.

siloxanes Compounds of general formula $H_3Si[OSiH_2]_nOSiH_3$, named 'disiloxane' (n = O), 'trisiloxane' (n = 1), etc.

siloxy (silyloxy) H_3SiO–

silthianes A variation of 'silathianes'

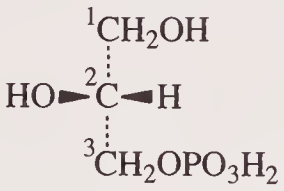
silyl H_3Si–

silylene H_2Si=

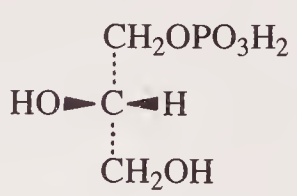
silylidyne HSi≡

sinapoyl [3-(4-hydroxy-3,5-dimethoxyphenyl)-1-oxo-2-propenyl]

sn- *sn-* (stereospecifically numbered) is used to indicate the configuration of glycerol derivatives. In *sn*-glycerol derivatives, the carbon atom which appears at the top of that Fischer projection showing a vertical chain with the OH group of C(2) to the left is designated as C(1)



sn-glycerol 3-phosphate



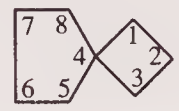
sn-glycerol 1-phosphate

sorboyl (1-oxo-2,4-hexadienyl) $H_3CCH{=}CHCH{=}CHCO$–

sphingoids Refers to sphingamine (D-*erythro*-2-amino-1,3-octadecanediol), its homologues, stereoisomers and derivatives. Important biochemicals

spiro compounds Spiro ring systems are polycyclic ring systems containing two rings or ring systems having only one atom in common; this common atom constitutes the only connection, direct or indirect, between the two rings or ring systems. Such common atoms are called 'spiro atoms'. Examples of types of names given to spiro compounds follow.

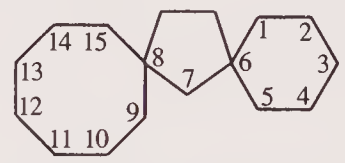
Spiro[3.4]octane. This name denotes that there is one spiro atom and a total of eight atoms (from octane) in the structure. The numbers in square brackets, [3.4], show that there are three atoms linked to the spiro atom in one ring and four atoms linked to the spiro atom in the other ring.



spiro[3.4]octane

Numbering starts with a ring atom next to the spiro atom and proceeds first around the smaller ring, then through the spiro atom, and then around the second ring. Heteroatoms are denoted by replacement nomenclature.

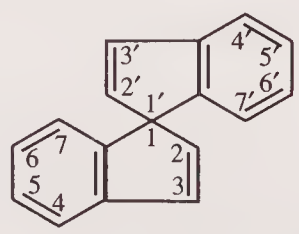
Dispiro[5.1.7.2]heptadecane. This name indicates that there are two spiro atoms and a total of 17 atoms in the structure. The numbers in square brackets, [5.1.7.2], are the numbers of skeletal atoms linked to the spiro atoms in the same order as the numbering proceeds about the ring. Thus, 5, 1, 7 and 2 correspond to atoms 1–5, 7, 9–15 and 16–17, respectively.



dispiro[5.1.7.2]heptadecane

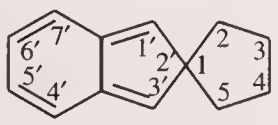
Numbering starts with a ring atom next to a terminal spiro atom and proceeds around this terminal ring so as to give the spiro atoms as low numbers as possible. Trispiro names, etc., are formed similarly.

*1,1′-Spirobiindene or 1,1′-spirobi[1*H*-indene]*. 'Spirobi' indicates that two similar components are joined through a spiro atom. The numbers of one component are distinguished by primes.



1,1′-spirobi[1*H*-indene]

*Spiro[cyclopentane-1,2′-[2*H*]indene].* This name shows that a cyclopentane ring is joined to a 2*H*-indene ring through a spiro atom at the 1 position of the cyclopentane and the 2 position of the indene. The numbers of the second component (indene) are distinguished by primes.



spiro[cyclopentane-1,2′-[2*H*]indene]

Alternatively, the term 'spiro' may be placed between the components. Thus, 'cyclopentane-spiro-2'-indene' and 'indene-2-spiro-1′-cyclopentane' are alternative names for the above compound.

SR- See *RS-*

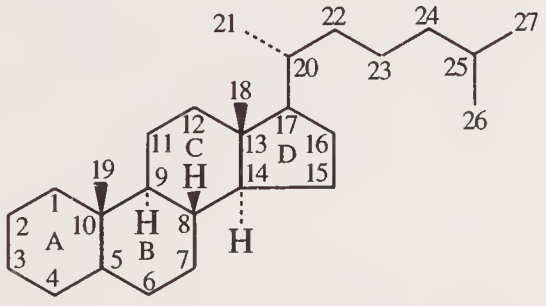
starburst dendrimer See dendrimer

stearoyl (1-oxooctadecyl) $H_3C(CH_2)_{16}CO–$

stearyl octadecyl $H_3C(CH_2)_{17}$

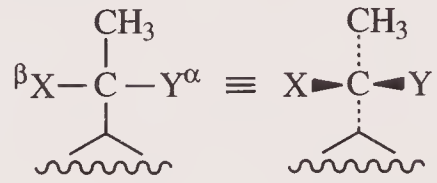
steroids Naturally occurring compounds and synthetic analogues based on the cyclopenta-[*a*]phenanthrene skeleton. Entries for the most important steroids (natural products, drugs and fundamental parents) are given in DOC 6. For a comprehensive treatment of naturally occurring steroids, see the *Dictionary of Steroids*. A few aspects of steroid nomenclature are covered here. For further details see the *Dictionary of Steroids* and also: *Pure. Appl. Chem.* 1989, **61**, 1783

Steroids are numbered and rings are lettered as follows:



The following steroid names are the ones usually used as parent names: androstane, bufanolide, campestane, cardanolide, cholane, cholestane, ergostane, estrane (oestrane), furostan, gonane, gorgostane, poriferastane, pregnane, spirostan and stigmastane. The structures of the most important members of these series are given in DOC 6.

Stereochemistry is denoted by α and β; ξ (xi) is used for positions of unknown stereochemistry. For a steroid structure drawn in the normal manner, α-denotes that a substituent projects below the plane of the paper and β- indicates that a substituent projects above the plane of the paper. At a ring junction position, it is the H or Me group that determines whether the configuration is α- or β-. The configuration of steroids at the ring junctions is assumed to be 8β,9α,10β,13β,14α unless otherwise stated. The configuration at position 5 is not assumed and should be specified as 5α– or 5β-. The side-chain at C(17) is normally 17β. In pregnane the stereochemistry at C(20) was formerly designated 20α or 20β based on a Fischer projection, as follows:



Terms used to describe modified steroid skeletons include: nor (shortening of a side-chain or contraction of a ring), homo (expansion of a ring), cyclo (formation of an additional ring), seco (fission of a ring) and abeo (migration of a bond).

stiba Replacement prefix denoting an antimony atom. For a full treatment of organoantimony compounds, see the *Dictionary of Organometallic Compounds*

styphnate An ester, salt or addition compound of styphnic acid (2,4,6-trinitro-1,3-benzenediol)

styryl (2-phenylethenyl) PhCH=CH–

suberoyl (1,8-dioxo-1,8-octanediyl) $–CO(CH_2)_6CO–$

substitutive nomenclature A substitutive name indicates the substitution of hydrogen by another atom or group. It is the commonest form of nomenclature

subtractive nomenclature A subtractive name implies the loss of certain atoms or groups from a parent structure. Examples are: de-*N*-methylmorpholine and 7,8-didehydrocholesterol

succinamoyl (4-amino-1,4-dioxobutyl) $H_2NCOCH_2CH_2CO–$

succinimido (2,5-dioxo-1-pyrrolidinyl)

succinyl (1,4-dioxo-1,4-butanediyl) $–COCH_2CH_2CO–$

sulfamino (sulfoamino) $HOSO_2NH–$

sulfamoyl or **sulfamyl** $H_2NSO_2–$

sulfane Compounds containing an unbranched chain of sulfur atoms may be named as disulfanes, trisulfanes, etc. Thus, phenyltrisulfane is PhSSSH

sulfanilyl [(4-aminophenyl)sulfonyl] 4-$H_2NC_6H_4SO_2$–

-sulfenamide Suffix denoting –SNH_2. Thus, ethanesulfenamide is $EtSNH_2$

sulfenamoyl H_2N–S–

-sulfenic acid Suffix denoting –S–OH

sulfeno HOS–

sulfhydryl mercapto HS–

sulfides Compounds R^1SR^2. Sulfur analogues of ethers. Thus, diethyl sulfide is Et_2S. R^1SSR^2 are disulfides, R^1SSSR^2 are trisulfides, etc. The word 'sulfide' is also used to denote addition of S= to a heteroatom as in phosphine sulfide (H_3P=S)

-sulfinamide Suffix denoting –S(O)NH_2

-sulfinamidine Suffix denoting –S(=NH)NH_2

sulfinamoyl $H_2NS(O)$–

sulfines *S*-Oxides of thiocarbonyl compounds, such as PhCO=SO

-sulfinic acid Suffix denoting –S(O)OH

-sulfinimidic acid Suffix denoting –S(=NH)OH

sulfino HOS(O)–

-sulfinohydrazonic acid Suffix denoting –S(=NNH_2)OH

-sulfinohydroximic acid Suffix denoting –S(=NOH)OH

sulfinyl OS=

sulfo HO_3S–

-sulfonamide Suffix denoting –SO_2NH_2

sulfones Compounds $R^1S(O)_2R^2$. Thus, dimethyl sulfone is $Me_2S(O)_2$

-sulfonic acid Suffix denoting –$S(O)_2OH$

-sulfonimidic acid Suffix denoting –S(O) (=NH)OH

sulfonio H_2S^+–

sulfonium H_3S^+

-sulfonohydrazide Suffix denoting –SO_2NHNH_2

-sulfonohydrazonic acid Suffix denoting –S(O) (=NNH_2)OH

-sulfonohydroximic acid Suffix denoting –S(O) (=NOH)OH

sulfonyl –SO_2–

sulfonylides Cyclic intermolecular esters of hydroxysulfonic acids. Analogues of lactides

sulfoxides Compounds $R^1S(O)R^2$. Thus, dimethyl sulfoxide is $Me_2S(O)$ (sometimes called methyl sulfoxide). Sulfoxides having two different alkyl groups are chiral (tetrahedral S atom)

sulfoxonium H_3S^+=O

sulfuryl sulfonyl –SO_2–

sulph- British variant spelling of sulf-. IUPAC now recommends 'sulf-'

sultams Cyclic esters of sulfonic acids. They contain the grouping –$S(O)_2N(R)$– as part of a ring

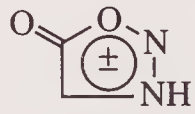
sultims Tautomeric forms of sultams. They contain –S(O)(OH)=N– as part of a ring

sultines Cyclic esters of hydroxysulfinic acids. They contain –S(O)O- as part of a ring

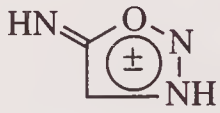
sultones Cyclic esters of hydroxysulfonic acids. Analogues of lactones. They contain the grouping –$S(O)_2O$– as part of a ring

supermesityl (2,4,6-tris (1,1-dimethylethyl) phenyl)

sydnones A class of compounds derived from 1,2,3-oxadiazolidin-5-one substituted in the 3 position by loss of two hydrogen atoms, resulting in a mesoionic system (see *mesoionic compounds*). 'Sydnone imines' are similar compounds derived from 1,2,3-oxadiazolidin-5-imine.



sydnone



sydnone imine

sym- Abbreviation for *symmetric(al)* as in *sym*-dichloroethane, $ClCH_2CH_2Cl$. Sometimes used to indicate 1,3,5-substitution in a benzene ring; e.g. *sym*-trichlorobenzene is 1,3,5-trichlorobenzene

syn- A stereochemical descriptor used for bridged bicyclic systems. In a bicyclo [*X. Y. Z*] compound ($X \geq Y > Z$), *syn*- denotes that a substituent on the *Z* bridge points towards the *X* bridge. For a diagram, see *anti*-. Also used for configuration of oximes, etc. (obsol.: use *E*/*Z*)

t- Abbreviation for *tertiary* as in *tert*-butyl

t- Abbreviation for *trans*-

-t Denotes tritium in the Boughton system of naming isotopically labelled compounds. See *labelled compounds*

talo- A configurational prefix used in carbohydrate nomenclature. See *carbohydrates*

tannins Plant polyphenols. For a comprehensive coverage, see the *Dictionary of Natural Products*

tartronoyl (2-hydroxy-1,3-dioxo-1,3-propanediyl) –COCH(OH)CO–

tauryl [(2-aminoethyl)sulfonyl] $H_2NCH_2CH_2SO_2$–

tellura Replacement prefix denoting tellurium

-tellurenamide Suffix denoting $-TeNH_2$

-tellurenic acid Suffix denoting –TeOH

tellureno HOTe–

tellurides Compounds R^1TeR^2, tellurium analogues of ethers

tellurilimine $H_2Te{=}NH$

-tellurinamide Suffix denoting $-Te(O)NH_2$

-tellurinic acid Suffix denoting –Te(O)OH

tellurino HOTe(O)–

telluro –Te– Used when the free valencies are attached to different atoms that are not otherwise connected

-telluronamide Suffix denoting $-Te(O)_2NH_2$

tellurones $R^1C(=Te)R_2$, tellurium analogues of ketones

-telluronic acid Suffix denoting $-Te(O)_2OH$

tellurono $HOTe(O)_2$–

telluroxo Te= Used when both free valencies are attached to the same atom

telluryl HTe–

ter Numerical prefix denoting 'three'. Used only in ring assembly names as in terphenyl. See *ring assemblies*

terephthaloyl (1,4-phenylenedicarbonyl) $1,4\text{-}C_6H_4(CO–)_2$

terpenoids A class of organic compounds, the common structural feature of which is a carbon skeleton of repeating isoprene units. Entries for a limited selection of the most important terpenoids are given in DOC 6. For a comprehensive treatment, see the *Dictionary of Natural Products*

tert- Abbreviation for *tertiary* as in *tert*-butyl

tetra Numerical prefix denoting 'four'. Tetracosa denotes '24', tetraconta denotes '40', and tetradeca denotes '14'

tetradecanoyl (1-oxotetradecyl) $H_3C(CH_2)_{12}CO–$

tetrakis Numerical prefix used instead of tetra with complex terms and to avoid ambiguity

tetramethylene 1,4-butanediyl $–(CH_2)_4–$

tetrapyrroles A general term for porphyrins and biline derivatives. For further information, see the *Dictionary of Natural Products*

thenoyl (thienylcarbonyl)

thenyl (thienylmethyl)

thenylidene (thienylmethylene)

thenylidyne (thienylmethylidyne)

thetins Inner sulfonium salts analogous to betaines, e.g. $Me_2S^+CH_2COO^-$

thexyl (1,1,2-trimethylpropyl) $(H_3C)_2CHC(CH_3)_2–$

thia Replacement prefix denoting a sulfur atom

-thial Suffix denoting –CHS at the end of an aliphatic chain. Thus, hexanethial is $H_3C(CH_2)_4CHS$

thieno The ring fusion prefix derived from thiophene

thienyl The radical derived from thiophene

thio Denotes replacement of oxygen by sulfur as in thiophenol, thiourea. Also, the multiplying radical –S–. Similarly, 'dithio' is –SS–, 'trithio' is –SSS–, etc.

thioacetals Sulfur analogues of acetals

thioaldehydes Sulfur analogues of aldehydes, RCHS

-thioamide Suffix denoting $-C(S)NH_2$ at the end of an aliphatic chain

(thiocarbamoyl) (aminothioxomethyl) $H_2NC(S)–$

(thiocarbonyl) carbonothioyl –C(S)–

thiocarboxylic acids Compounds RC(S)OH, RC(O)SH and RC(S)SH, sulfur analogues of carboxylic acids

thiocyanates Compounds RSCN. Thus, methyl thiocyanate is MeSCN

thiocyanato NCS–

thiocyano thiocyanato NCS–

-thioic acid Suffix denoting –C(S)OH (-thioic *O*-acid) or –C(O)SH (-thioic *S*-acid) at the end of an aliphatic chain; '-dithioic acid' denotes –C(S)SH

thioketones Sulfur analogues of ketones

-thiol Suffix denoting –SH. 'Thiols' are compounds RSH

thiolates Metal derivatives of thiols. Thus, sodium ethanethiolate is EtSNa

-thione Suffix denoting a thioketone. Thus, 2-butanethione is $H_3CC(=S)CH_2CH_3$

thionia Replacement prefix for a positively charged sulfur atom

thionyl sulfinyl –S(O)–

thiophenol Benzenethiol, PhSH. In order to avoid confusion, hydroxythiophene is called thiophene-ol

thiouronium salts Quaternary derivatives of thiourea (isothiourea) with structure $[RSC(=NH)NH_2]^+ X^-$

thioxo S= Used when both free valencies are attached to the same atom

-thioyl Suffix denoting an acyl radical derived from a thioic acid

thiuronium salts See *thiouronium salts*

threo- A configurational prefix. See *carbohydrates*. Can be used generally to denote stereoisomers having the threose-like configuration. Ambiguity can occur

threonyl $H_3CCH(OH)CH(NH_2)CO–$ The acyl radical from threonine used in naming peptides

tigloyl (*E*)-(2-methyl-1-oxo-2-butenyl) (*E*)-$H_3CCH{=}C(CH_3)CO–$ The (*Z*)-form is 'angeloyl'

toloxy (methylphenoxy) $H_3CC_6H_4O–$

toluidino [(methylphenyl)amino] $H_3CC_6H_4NH–$

toluidides *N*-(Methylphenyl) amides. They may be named analogously to anilides. Thus, aceto-*m*-toluidide is $H_3CCONHC_6H_4CH_3$-3

toluoyl or **toluyl** (methylbenzoyl) $H_3CC_6H_4CO–$

tolyl (methylphenyl) $H_3CC_6H_4–$

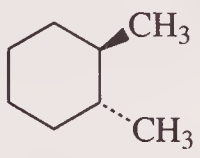
α-tolyl (phenylmethyl) $PhCH_2–$

tolylene (methylphenylene) $–(H_3CC_6H_3)–$

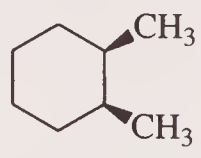
tosyl [(4-methylphenyl)sulfonyl] 4-$H_3CC_6H_4SO_2–$

tosylate or **tosate** An ester of *p*-toluenesulfonic acid

trans- Stereochemical descriptor denoting that two atoms or groups are on the opposite side of a ring.

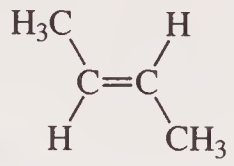


trans-1,2-dimethylcyclohexane

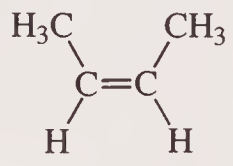


cis-

Also used to indicate the configuration about a double bond. (*E*)- and (*Z*)- are now more commonly used instead of *cis*- and *trans*-



trans-2-butene
(*E*)-2-butene



cis-2-butene
(*Z*)-2-butene

tri Numerical prefix denoting 'three'. Triaconta denotes '30', tricosa denotes '23', and trideca denotes '13'

tricyclo For an explanation of names like tricyclo[5.1.0.$0^{3,5}$]octane, see *von Baeyer nomenclature*

tridecanoyl (1-oxotridecyl) $H_3C(CH_2)_{11}CO–$

triflyl [(trifluoromethyl)sulfonyl] $F_3CSO_2–$

trimethylene 1,3-propanediyl $–(CH_2)_3–$

tris Numerical prefix used instead of tri with complex terms and to avoid ambiguity

triterpenoids Terpenoids having a C_{30} skeleton. Entries for a limited selection of the most important triterpenoids are given in DOC 6. For a comprehensive treatment, see the *Dictionary of Natural Products*

tritio T– Indicates replacement of a hydrogen atom by a tritium atom

trityl (triphenylmethyl) $Ph_3C–$

tropoyl (3-hydroxy-1-oxo-2-phenylpropyl) $PhCH(CH_2OH)CO–$

tryptophyl The acyl radical from tryptophan used in naming peptides

tyrosyl 4-$HOC_6H_4CH_2CH(NH_2)CO–$ The acyl radical from tyrosine used in naming peptides

ulosaric acids, ulosonic acids, ulosuronic acids Acids derived from the oxidation of ketoses. Names are formed by changing the '-ose' ending of the ketose name to '-ulosaric acid', '-ulosonic acid' and '-ulosuronic acid'. See *carbohydrates*

-ulose Denotes a ketose; '-ulofuranose' and '-uropyranose' denote a ketose in the cyclic hemiacetal form having five- and six-membered rings, respectively

undeca Numerical prefix denoting '11'

undecanoyl (1-oxoundecane) $H_3C(CH_2)_9CO–$

unsym- Abbreviation for *unsymmetrical* as in *unsym*-dichloroethane, H_3CCHCl_2. Sometimes used to indicate 1,2,4-substitution on a benzene ring; e.g. *unsym*-trichlorobenzene is 1,2,4-trichlorobenzene

ureido [(aminocarbonyl)amino] $H_2NCONH–$

urethanes Esters of carbamic acid. Urethane itself is ethyl carbamate and hence phenylurethane is PhNHCOOEt

ureylene (carbonyldiimino) $–NHC(O)NH–$

uronic acids Monocarboxylic acids derived by oxidation of the terminal CH_2OH of aldoses. Names are formed by replacing the '-ose' ending of the aldose name by '-uronic acid'. See *carbohydrates*

uronium salts Quaternary derivatives of urea (isourea) with structure $[ROC(=NH_2)NH_2]^+ X^-$

v- Abbreviation for *vicinal* as in *v*-triazine (1,2,3-triazine)

valeryl (1-oxopentyl) $H_3C(CH_2)_3CO–$

valyl $(H_3C)_2CHCH(NH_2)CO–$ The acyl radical from valine used in naming peptides

vanilloyl (4-hydroxy-3-methyoxybenzoyl)

vanillyl [(4-hydroxy-3-methoxyphenyl)methyl]

veratroyl (3,4-dimethoxybenzoyl) $3,4\text{-}(MeO)_2C_6H_4CO–$

***o*-veratroyl** (2,3-dimethoxybenzoyl) $2,3\text{-}(MeO)_2C_6H_4CO–$

veratryl [(3,4-dimethoxyphenyl)methyl] $3,4\text{-}(MeO)_2C_6H_4CH_2–$

vic- Abbreviation for *vicinal*. Sometimes used to indicate 1,2,3-substitution on a benzene ring; e.g. *vic*-trichlorobenzene is 1,2,3-trichlorobenzene

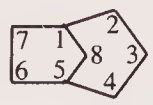
vinyl ethenyl $H_2C{=}CH–$

vinylene 1,2-ethenediyl –CH=CH–

vinylidene ethenylidene $H_2C{=}C{=}$

von Baeyer nomenclature von Baeyer names are used mostly for bridged ring systems and occasionally for non-bridged systems. Examples of von Baeyer names are: bicyclo[3.2.1]octane and tricyclo[7.4.1.$0^{3,6}$]tetradecane.

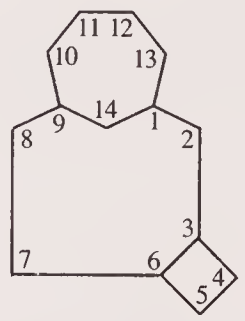
Bicyclo[3.2.1]octane. 'Bicyclo' denotes two rings and 'octane' denotes a total of eight skeletal atoms in the ring system. '[3.2.1]' gives the sizes of the three bridges connecting two bridgehead atoms.



bicyclo[3.2.1]octane

The system is numbered starting from one of the bridgeheads and numbering by the longest possible path to the second bridgehead; numbering is then continued via the longer unnumbered path back to the first bridgehead and is completed via the third bridge.

Tricyclo[7.4.1.$0^{3,6}$]tetradecane. 'Tricyclo' denotes three rings and 'tetradecane' denotes a total of 14 skeletal atoms in the ring system. '[7.4.1]' gives the sizes of three bridges connecting two bridgehead atoms as in the previous example; these three bridges are numbered as in the previous example. '$0^{3,6}$' denotes that there is a bridge of zero atoms (i.e. a bond) between the atoms numbered 3 and 6.



Heterocyclic systems are named by replacement nomenclature. Unsaturation is denoted by '-ene' and '-yne' suffixes. For more information, see Eckroth, D. R., *J. Org. Chem.*, 1967, **32**, 3312

xanthic acids *O*-Esters of carbonodithioic acid, ROC(S)SH. Thus, ethylxanthic acid is EtOC(S)SH. 'Xanthates' are salts of xanthic acids

xanthyl Contracted form of xanthenyl

xenyl (1,1′-biphenyl)yl $PhC_6H_4–$

xylidides *N*-(Dimethylphenyl) amides. They may be named analogously to anilides. Thus, aceto-2,4-xylidide is $CH_3CONHC_6H_3(CH_3)_2$-2,4

xylidino [(dimethylphenyl)amino] $(H_3C)_2C_6H_3NH–$

xylo- A configurational descriptor used in carbohydrate nomenclature. See *carbohydrates*

xyloyl (dimethylbenzoyl) $(H_3C)_2C_6H_3CO–$

xylyl (dimethylphenyl) $(H_3C)_2C_6H_3–$

xylylene [phenylenebis(methylene)] $–CH_2C_6H_4CH_2–$

-yl Suffix denoting a univalent radical

-ylene Suffix denoting a bivalent radical in which the free valencies are on different atoms

-ylidene Suffix denoting a bivalent radical in which the free valencies are on the same atom

ylides Compounds in which an anionic site is attached directly to a heteroatom carrying a positive charge; e.g. triphenylphosphonium methylide is $Ph_3P^{\oplus}–CH^{\ominus}$

-ylidyne Suffix denoting a trivalent radical in which the free valencies are on the same atom

ylium Suffix denoting a carbonium atom; e.g. methylium is H_3C^+, acetylium is $H_3CC^+(=O)$

-yne Ending denoting the presence of a triple bond

Z- A stereochemical descriptor for denoting the configuration at a double bond. See *E-*

z Equivalent to ***Z*** in denoting configuration at a single bond exhibiting restricted rotation (*Beilstein*)

zwitterionic compounds Another term for betaines or inner salts

8.3 Acronyms in organic chemistry

Based on Daub, G.H., *et al.*, *Aldrichimica Acta*, 1984, **17**, no. 1 (reproduced with permission), with some expansion.

Notes

- Not all of the acronyms given here are to be found in the DOC 6 indexes, although most of the compounds referred to are in DOC 6 or one of its companion publications (e.g. *Dictionary of Organometallic Compounds*). This is deliberate policy because of the proliferation of acronyms resulting in frequent duplications. This list should therefore be used with caution.
- Some acronyms are based on obsolete or misleading nomenclature, e.g. DMPU (standing for *N*,*N*′-dimethylpropyleneurea) = 1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone.
- See also the lists of abbreviations for amino acids given in Section 8.2 (Tables 8.1 and 8.2).
- The standard work on protective groups is *Protective Groups in Organic Synthesis*, T.W. Greene and P.G.M. Wuts, 2nd edn, Wiley-Interscience, 1991.

AA	anisylacetone
AAA	acetoacetanilide
AAAF	2-(*N*-acetoxyacetylamino)fluorene
AAMX	acetoacet-*m*-xylidide (*m*-aceto-acetoxylidide)
AAO	acetaldehyde oxime
AAOA	acetoacet-*o*-anisidide (*o*-aceto-acetanisidide)
AAOC	acetoacet-*o*-chloroanilide (*o*-aceto-acetochloranilide)
AAOT	acetoacet-*o*-toluidide (*o*-aceto-acetotoluidide)
ABA	abscisic acid
ABL	α-acetyl-γ-butyrolactone
ABTS	2,2′-azinobis(3-ethylbenzo-thiazoline-6-sulfonic acid)
Ac	acetate
Ac	acetyl
7-ACA	7-aminocephalosporanic acid
ACAC (acac)	acetylacetonate
ACES	*N*-(2-acetamido)-2-aminoethane-sulfonic acid
Acm	acetamidomethyl
ACTH	adrenocorticotropic hormone
Ad	adamantyl
ADA	*N*-(2-acetamido)iminodiacetic acid [*N*-(carbamoylmethyl)-iminodiacetic acid]
7-ADCA	7-aminodesacetoxycephalosporanic acid
ADDC	ammonium diethyldithiocarbamate
ADMA	alkyldimethylamine
Adoc	1-adamantyloxycarbonyl
ADP	adenosine 5′-diphosphate
Adpoc	1-(1-adamantyl)-1-methylethoxy-carbonyl
AEP	1-(2-aminoethyl)piperazine
AET	*S*-2-aminoethylisothiouronium bromide hydrobromide
AIBN	2,2′-azobisisobutyronitrile
AICA	5(4)-aminoimidazole-4(5)-carboxamide
AIP	aluminium isopropoxide
Ala	alanine
Alloc	allyloxycarbonyl
Am	amyl
AMBA	3-amino-4-methoxybenzanilide
AMEO	3-aminopropyltriethoxysilane
AMMO	2-aminopropyltrimethoxysilane
AM-ex-OL	4-chloro-2-phenylquinazoline
bis-AMP	*N*-bis(hydroxyethyl)-2-amino-2-methyl-1-propanol
AMP	adenosine 5′-monophosphate
AMPD	2-amino-2-methyl-1,3-propanediol
AMPS	2-acrylamido-2-methylpropane-sulfonic acid
AMTCS	amyltrichlorosilane
AN	acetonitrile
ANM	*N*-(4-anilino-1-naphthyl)maleimide
ANPP	4-azido-2-nitrophenyl phosphate
ANS-NH4	8-anilinonaphthalene-1-sulfonic acid, ammonium salt
ANT	(see AN)
AOC	allyloxycarbonyl
AOM	*p*-anisyloxymethyl
APAD	3-acetylpyridine adenine dinucleotide

APAP	*N*-acetyl-*p*-aminophenol
APDC	ammonium 1-pyrrolidine-carbodithioate
APDTC	ammonium 1-pyrrolidinedithio-carbamate
APG	*p*-azidophenylglyoxal hydrate
p-APMSF	(*p*-amidinophenyl)methyl-sulfonyl fluoride
APS	adenosine 5′-phosphosulfate
APTP	*N*-(4-azidophenylthio)phthalimide
Ar	aryl
Arg	arginine
ASC	*p*-acetylaminobenzenesulfonyl chloride
ATA	anthranilamide
ATC	ethyltrichlorosilane
ATEE	*N*-acetyl-L-tyrosine ethyl ester monohydrate
ATP	adenosine 5′-triphosphate
BA	benzyladenine
BAA	*N*-α-benzoyl-L-argininamide hydrochloride monohydrate
1,3-BAC	1,3-bis(aminomethyl)cyclohexane
BAEE	*N*-α-benzoyl-L-arginine ethyl ester
BAL	2,3-dimercapto-1-propanol (British anti-Lewisite)
BAME	*N*-α-benzoyl-L-arginine methyl ester
BANA	*N*-α-benzoyl-DL-arginine-2-naphthylamide
BANI	*N*-α-benzoyl-DL-arginine-4-nitroanilide
BAO	bis(4-aminophenyl)-1,3,4-oxadiazole
BaP (BAP)	benzo[*a*]pyrene
BAP	benzylaminopurine
BAPNA	*N*-α-benzoyl-DL-arginine-*p*-nitroanilide hydrochloride
9-BBN	9-borabicyclo[3.3.1]nonane
BBO	2,5-bis(4-biphenylyl)oxazole
BBOD	2,5-bis(4-biphenylyl)-1,3,4-oxadiazole
BBOT	2,5-bis(5-*tert*-butyl-2-benzoxazolyl)thiophene
BBP	benzyl butyl phthalate
BCA	*N*-benzylcyclopropylamine
BCB	bromocresol blue
BCDC	*N*-benzylcinchonidinium chloride
BCG	bromocresol green
BCNC	(+)-*N*-benzylcinchonidinium chloride
BCNU	1,3-bis(2-chloroethyl)-1-nitrosourea
BCP	bromocresol purple
BCP	butyl carbitol piperonylate
BCPB	bromochlorophenol blue
BCPC	*sec*-butyl *N*-(3-chlorophenyl)-carbamate
BDCS	(see TBSCl)
t-BDEA	*tert*-butyldiethanolamine
BDMA	benzyldimethylamine
BDPA	α,γ-bisdiphenylene-β-phenylallyl, free radical
BDT	1,3-benzodithiolan-2-yl
BES	*N*,*N*-bis(2-hydroxyethyl)-2-amino-ethanesulfonic acid
BGE	butyl glycidyl ether
BHA	3-*tert*-butyl-4-hydroxyanisole
BHC	benzene hexachloride
BHMF	2,5-bis(hydroxymethyl)furan
BHMT	bis(hexamethylene)triamine
BHT	2,6-di-*tert*-butyl-4-methylphenol (butylated hydroxytoluene)
BIC	5-benzisoxazolylmethoxycarbonyl
BICINE	*N*,*N*-bis(2-hydroxyethyl)glycine
BINAP	2,2′-bis(diphenylphosphino)-1,1′-binaphthyl
bis-MSB	*p*-bis(*o*-methylstyryl)benzene
Bis-Tris	2,2-bis(hydroxymethyl)-2,2′,2″-nitrilotriethanol [bis(2-hydroxy-ethyl)aminotris(hydroxymethyl)-methane]
BLO	γ-butyrolactone
Bmpc	2,4-dimethylthiophenoxycarbonyl
Bmpm	1,1-bis(4-methoxyphenyl)-1-pyrenylmethyl
BMS	borane–methyl sulfide complex
Bn	benzyl (also Bzl or Bnz)
BN	benzonitrile
BNAH	1-benzyl-1,4-dihydronicotinamide
BNB	2,4,6-tri-*tert*-butylnitrosobenzene
Bnz	(see Bn)
BOC (or Boc)	*tert*-butoxycarbonyl
t-BOC	(see BOC)
BOC-ON	2-(*tert*-butoxycarbonyloxyimino)-2-phenylacetonitrile
BOC-OSU	*N*-(*tert*-butoxycarbonyloxy)-succinimide
BOC-OTCP	*tert*-butyl 2,4,5-trichlorophenyl carbonate

BOM	benzyloxymethyl
BON	β-hydroxynaphthoic acid
BOP	benzotriazol-1-yloxytris(dimethylamino)phosphonium hexafluorophosphate
BPB	bromophenol blue
BPBG	butyl phthalyl butyl glycolate
BPC	n-butylpyridinium chloride
BPCC	2,2′-bipyridinium chlorochromate
BPO	2-(4-biphenylyl)-5-phenyloxazole
Bpoc	1-methyl-1-(4-biphenylyl)-ethoxycarbonyl
BPPM	(2*S*,4*S*)-*N*-*tert*-butoxycarbonyl-4-diphenylphosphino-2-diphenylphosphinomethylpyrrolidine
BPR	bromophenol red
BSA	*N*,*O*-bis(trimethylsilyl)acetamide
BSC	*N*,*O*-bis(trimethylsilyl)carbamate
BSH	benzenesulfonyl hydrazide
BSOCOES	bis[2-(succinimidooxycarbonyloxy)ethyl] sulfone
BST chloride	2-(2-benzothiazolyl)-5-styryl-3-(4-phthalhydrazidyl)-tetrazolium chloride
BSTFA	*N*,*O*-bis(trimethylsilyl)trifluoroacetamide
BT	blue tetrazolium
Bt	1-benzotriazolyl
BTA	benzotrifluoroacetone
BTB	bromothymol blue
BTDA	3,3′,4,4′-benzophenonetetracarboxylic dianhydride
BTEAC	benzyltriethylammonium chloride
BTEE	*N*-benzoyl-L-tyrosine ethyl ester
BTFA	bis(trifluoroacetamide)
BTMSA	bis(trimethylsilyl)acetylene
Bu	butyl
nBu	n-butyl
iBu	isobutyl
sBu	*sec*-butyl
tBu	*tert*-butyl
Bum	*tert*-butoxymethyl
t-Bumeoc	1-(3,5-di-*tert*-butylphenyl)-1-methylethoxycarbonyl
Bz	benzoyl
Bzh	diphenylmethyl (benzhydryl)
Bzl	benzyl
Cam	carboxamidoethyl
CAN	ceric ammonium nitrate
CAP	cellulose acetate phthalate
CAP-Li_2	carbamoyl phosphate, dilithium salt
CAPS	3-cyclohexylamino-1-propanesulfonic acid
CAT	2-chloro-4,6-bis(ethylamino)-*s*-triazine
Cathyl	ethoxycarbonyl (or carbethoxy)
p-CBA	*p*-carboxybenzaldehyde
CBC	carbomethoxybenzenesulfonyl chloride
Cbm	carbamoyl
CBn (or Cb)	benzyloxycarbonyl (or carbobenzoxy)
Cbz (or CBZ)	(see CBn)
CBZ-HONB	*N*-benzyloxycarbonyloxy-5-norbornene 2,3-dicarboximide
CCH	cyclohexylidenecyclohexane
CCNU	1-(2-chloroethyl)-3-cyclohexyl-1-nitrosourea
CD	cyclodextrin
CDAA	chlorodiallylacetamide
CDC	cycloheptaarylose–dansyl chloride complex
CDEC	2-chloroallyl *N*,*N*-diethyldithiocarbamate
CDP	cytidine 5′-diphosphate
CDTA	*trans*-1,2-diaminocyclohexane-*N*,*N*,*N*′,*N*′-tetraacetic acid
CE	cyanoethyl
Cee	1-(2-chloroethoxy)ethyl
CEEA	*N*-(2-cyanoethyl)-*N*-ethylamine
CEEMT	*N*-(2-cyanoethyl)-*N*-ethyl-*m*-toluidine
CEMA	*N*-(2-cyanoethyl)-*N*-methylaniline
CEPEA	*N*-(2-hydroxyethyl)-*N*-(2-cyanoethyl)aniline
CF	5(6)-carboxyfluorescein
CHAPS	3-[(3-cholamidopropyl)dimethylammonio]propanesulfonate
CHES	2-(cyclohexylamino)ethanesulfonic acid
CHP	*N*-cyclohexyl-2-pyrrolidone
CHT	cycloheptatriene
5-CIA	5-chloroisatoic anhydride
CMA	carbomethoxymaleic anhydride
CMC	carboxymethyl cellulose
CMC	1-cyclohexyl-3-(2-morpholinoethyl)carbodiimide
CMDMCS	(chloromethyl)dimethylchlorosilane
CMP	cytidine 5′-monophosphate

CMPI	2-chloro-1-methylpyridinium chloride
CNT	cyanotoluene
CoA	coenzyme A
Coc	cinnamyloxycarbonyl
COD	cyclooctadiene
COT	cyclooctatetraene
Cp (or cp)	cyclopentadienyl
Cp* (or cp*)	pentamethylcyclopentadienyl
6-CP	6-chloropurine
4-CPA	4-chlorophenoxyacetic acid
m-CPBA	*m*-chloroperoxybenzoic acid
CPR	chlorophenol red
CPTEO	3-chloropropyltriethoxysilane
CPTMO	3-chloropropyltrimethoxysilane
CPTr	4,4′,4″-tris(4,5-dichlorophthalimido)triphenylmethyl
CSA	camphorsulfonic acid
CSI	chlorosulfonyl isocyanate
CTA	citraconic anhydride
CTAB (or CTABr)	cetyltrimethylammonium bromide
CTACl	cetyltrimethylammonium chloride
CTACN	cetyltrimethylammonium cyanide
CTAOH	cetyltrimethylammonium hydroxide
CTMP	1-[(2-chloro-4-methylphenyl)-4-methoxy-4-piperidinyl]
CTP	cytidine 5′-triphosphate
CYAP	*O*,*O*-dimethyl *O*-(*p*-cyanophenyl) phosphorothioate
cyclam	1,4,8,11-tetraazacyclotetradecane
cyclic AMP	adenosine 3′,5′-cyclic monophosphoric acid
CYP	*p*-cyanophenyl ethyl phenylphosphonothioate
CySH	cysteine
D	2,2′-dithiodibenzoic acid
2,4-D	2,4-dichlorophenoxyacetic acid
DAA	diacetone alcohol
DAA	diacetone acrylamide
DAB	*p*-dimethylaminoazobenzene
DAB	diaminobenzidine (usually 3,3′)
DABCO (or TED)	1,4-diazabicyclo[2.2.2]octane
DABITC	4-(*N*,*N*-dimethylamino)-azobenzene-4′-isothiocyanate
DABS-Cl	4-(*N*,*N*-dimethylamino)-azobenzene-4′-sulfonyl chloride
3,5-DACB	3,5-diaminochlorobenzene
DACH	*trans*-1,2-diaminocyclohexane
DACM-3	*N*-(7-dimethylamino-4-methyl-3-coumarinyl)maleimide
DAD	(see DEAD)
DAM	di(4-methoxyphenyl)methyl
DAMN	diaminomaleonitrile
DANSYL	5-dimethylaminonaphthalene-1-sulfonyl
DAP	diammonium phosphate
DAP	diallyl phthalate
DAPI	4′,6-diamidino-2-phenylindole dihydrochloride
DAS	4,4′-diaminostilbene-2,2′-disulfonic acid
DAST	diethylaminosulfur trifluoride
DATMP	diethylaluminium 2,2,6,6-tetramethylpiperidide
2,4-DB	2,4-dichlorophenoxybutyric acid
DBA	dibenz[*a*,*h*]anthracene
DBC·Br_2	dibenzo-18-crown-6/Br_2
DBCP	1,2-dibromo-3-chloropropane
DBDPO	decabromodiphenyl ether
DBD-Tmoc	2,7-di-*tert*-butyl [9-(10,10-dioxotetrahydroxanthyl)]-methylcarbonyl
DBIC	dibutylindolocarbazole
DBMIB	dibromomethylisopropylbenzoquinone
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBN	*p*,*p*′-dinitrobenzhydryl
DBP	dibutyl phthalate
DBPC	2,6-di-*tert*-butyl-*p*-cresol
DBS	dibutyl sebacate
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
2,4-DCAD	2,4-dichlorobenzaldehyde
DCAF	2′,4′-bis[di(carboxymethyl)aminomethyl]fluorescein
DCB	dicyanobenzene
2,4-DCBA	2,4-dichlorobenzoic acid
2,4-DCBC	2,4-dichlorobenzyl chloride
2,4′-DCBP	2,4′-dichlorobenzophenone
2,4-DCBTF	2,4-dichlorobenzotrifluoride
3,4-DCBTF	3,4-dichlorobenzotrifluoride
DCC	dicyclohexylcarbodiimide
DCCI	(see DCC)
DCEE	dichloroethyl ether
DCHA	dicyclohexylamine
DCHBH	dicyclohexylborane
DCI-HCl	1-(3′,4′-dichlorophenyl)-2-isopropylaminoethanol hydro chloride
DCM	dichloromethane

DCOC	2,4-dichlorobenzoyl chloride
DCPD	dicyclopentadiene
2,4-DCT	2,4-dichlorotoluene
3,4-DCT	3,4-dichlorotoluene
2,4-DCTC	2,4-dichlorobenzotrichloride
3,4-DCTC	3,4-dichlorobenzotrichloride
DCU	*N*,*N*-dichlorourethane
DDA	4,4′-dichlorodiphenylacetic acid
DDB	2,3-dimethoxy-1,4-bis(dimethylamino)butane
DDD	2,2′-dihydroxy-6,6′-dinaphthyl disulfide
o,*p*′-DDD	1-(*o*-chlorophenyl)-1-(*p*-chlorophenyl)-2,2-dichloroethane
p,*p*′-DDD	2,2-bis(*p*-chlorophenyl)-1,1-dichloroethane
o,*p*′-DDE	1-(*o*-chlorophenyl)-1-(*p*-chlorophenyl)-2,2-dichloroethylene
p,*p*′-DDE	2,2-bis(*p*-chlorophenyl)-1,1-dichloroethylene
DDH	1,3-dibromo-5,5-dimethylhydantoin
DDM	4,4′-dichlorodiphenylmethane
DDM	diphenyldiazomethane
DDMU	4,4′-dichlorodiphenyl-2-chloroethylene
DDOH	4,4′-dichlorodiphenylethanol
DDP	dichlorodiammineplatinum
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DDS	*p*,*p*′-diaminodiphenyl sulfone
DDS	dihydroxydiphenyl sulfone
DDSA	dodecenylsuccinic anhydride
o,*p*′-DDT	1-(*o*-chlorophenyl)-1-(*p*-chlorophenyl)-2,2,2-trichloroethane
p,*p*′-DDT	1,1-bis(*p*-chlorophenyl)-2,2,2-trichloroethane
DDVP	dimethyl 2,2-dichlorovinyl phosphate
DDZ	α,α-dimethyl-3,5-dimethoxybenzyloxycarbonyl
DEA	*N*,*N*-diethylaniline
DEAA	*N*,*N*-diethylacetoacetamide
DEAC	diethylaluminium chloride
DEAD	diethyl azodicarboxylate
DEAE-cellulose	diethylaminoethyl cellulose
DEAH	diethylaluminium hydride
DEAI	diethylaluminium iodide
DEAP	2,2-diethoxyacetophenone
DEASA	*N*,*N*-diethylaniline-3-sulfonic acid
DEC	2-diethylaminoethyl chloride hydrochloride
DEDM	diethyl diazomalonate
DEII	diethylindoloindole
DEIPS	2-(1,3-dithianyl)methyl
DEP	diethyl phthalate
DEP	diethyl pyrocarbonate
DEPC	diethylphosphoryl cyanide
DEPHA	di-(2-ethylhexyl)phosphoric acid
DESS	diethyl succinylsuccinate
DET	diethyl tartrate
DFP	diisopropyl fluorophosphate
DHA	dehydroacetic acid
DHA	9,10-dihydroanthracene
DHBA	3,4-dihydroxybenzylamine hydrobromide
DHBP	dihydroxybenzophenone (usually 4,4′)
DHEBA	1,2-dihydroxyethylene-bisacrylamide
DHET	dihydroergotoxine
DHN	5,12-dihydronaphthacene
DHP	diheptyl phthalate
DHP	dihydropyran
DIAD	diisopropyl diazodicarboxylate
DIB	1,3-diphenylisobenzofuran
DIBAC	diisobutylaluminium chloride
DIBAH	diisobutylaluminium hydride
DIBAL	(see DIBAH)
DIBAL-H	(see DIBAH)
DIC	(dimethylamino)isopropyl chloride hydrochloride
DIDP	diisodecyl phthalate
DI-ET	*N*,*N*-diethyl-*p*-phenylenediamine monohydrochloride
Diglyme	diethylene glycol dimethyl ether
DiHPhe	2,5-dihydroxyphenylalanine
Dimsyl Na	sodium methylsulfinylmethide
DIOP	2,3-*O*-isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphino)butane
DIPC	2-dimethylaminoisopropyl chloride hydrochloride
DIPEA	diisopropylethylamine
Diox	dioxane
DIPHOS	ethylenebis(diphenylphosphine)
DIPSO	3-[bis(2-hydroxyethyl)amino]-2-hydroxy-1-propanesulfonic acid
DIPT	diisopropyl tartrate
DITC	1,4-phenylene diisocyanate

DMA	*N*,*N*-dimethylaniline
DMA	dimethylacetamide
2,6-DMA	2,6-dimethylanisole
DMAA	*N*,*N*-dimethylacetoacetamide
DMAC	(see DMA, dimethylacetamide)
DMAD	dimethyl acetylenedicarboxylate
DMA-DEA	*N*,*N*-dimethylacetamide diethyl acetal
DMAEMA	2-dimethylaminoethyl methacrylate
DMAP	dimethylaminopropylamine
DMAP	4-dimethylaminopyridine
DMAPMA	dimethylaminopropyl methacrylamide
DMB	4,4′-dichloro-α-methylbenzhydrol
DMC	2-(dimethylamino)ethyl chloride
DMCS	dimethylchlorosilane
DMDAAC	dimethyldiallylammonium chloride
DME	1,2-dimethoxyethane (glyme)
DMECS	dimethylethylchlorosilane
DMEU	*N*,*N*′-dimethylethyleneurea
DMF	dimethylformamide
DMF-DMA	dimethylformamide dimethyl acetal
DMI	1,3-dimethyl-2-imidazolidinone
DMIPS	dimethylisopropylsilyl
Dmoc	dithianylmethoxycarbonyl
Dmp	dimethylphosphinyl
DMP	dimethyl phthalate
DMP	dimethyl pyrocarbonate
DMP	2,2-dimethoxypropane
2,6-DMP	2,6-dimethylphenol
DMP-30	2,4,6-tris(dimethylaminomethyl)-phenol
DMPA	2,2-dimethoxy-2-phenyl-acetophenone
DMPC	3-dimethylaminopropyl chloride hydrochloride
DMPE	1,2-bis(dimethylphosphino)ethane
DMPM	3,4-dimethoxybenzyl
DMPO	5,5-dimethyl-1-pyrroline *N*-oxide
DMPP	1,1-dimethyl-4-phenylpiperazinium iodide
DMPS	2,3-dimercapto-1-propanesulfonic acid (sodium salt)
DMPU	*N*,*N*′-dimethylpropyleneurea
DMS	4,6-dimethoxybenzene-1,3-disulfonyl chloride
DMS	dimethyl sulfide
DMSO	dimethyl sulfoxide
DMSS	dimethyl succinylsuccinate
DMT	dimethyl tartrate
DMT	dimethyl terephthalate
DMTD	2,5-dimercapto-1,3,4-thiadiazole
DMTr	di(*p*-methoxyphenyl)phenylmethyl
DMTSF	dimethyl(methylthio)sulfonium fluoroborate
DMTST	dimethyl(methylthio)sulfonium trifluoromethanesulfonate
DNA	deoxyribonucleic acid
DNAP	4-(2,4-dinitrophenylazo)-9-phenanthrol
DNB	*p*,*p*′-dinitrobenzhydryl
DNBS	2,4-dinitrobenzenesulfonic acid
DNBSC	2,4-dinitrobenzenesulfenyl chloride
DNF	2,4-dinitrofluorobenzene
DNFA	2,4-dinitro-5-fluoroaniline (Bergmann's reagent)
DNFB	(see DNF)
DNMBS	4-(4,8-dimethoxynaphthylmethyl)-benzenesulfonyl
DNP	2,4-dinitrophenyl
DNP	2,4-dinitrophenylhydrazone
DNP	dinonyl phthalate
DNPBA	3,5-dinitroperoxybenzoic acid
2,6-DNPC	2,6-dinitro-*p*-cresol
Dnp-F	(see DNF)
DNPF	(see DNF)
DNS	5-dimethylamino-1-naphthalene-sulfonic acid
DNS	4,4′-dinitrostilbene-2,2′-disulfonic acid, disodium salt
DNS-BBA	*N*-dansyl-3-aminobenzeneboronic acid
DNSA	5-dimethylaminonaphthalene-1-sulfonamide
DNTC	4-dimethylamino-1-naphthyl isothiocyanate
DOA	dioctyl adipate
Dobz	*p*-(dihydroxyboryl)benzyloxy-carbonyl
DOCA	deoxycorticosterone acetate
DOP	dioctyl phthalate
DOPA	3-(3,4-dihydroxyphenyl)-DL-alanine
DOPET	3,4-dihydroxyphenethyl alcohol
DOPS	DL-*threo*-3,4-dihydroxyphenyl-serine
2,4-DP	2,4-dichlorophenoxypropionic acid
DPB	1,4-diphenyl-1,3-butadiene
DPDM	diphenyl diazomalonate
DPH	1,6-diphenyl-1,3,5-hexatriene
DPM	diphenylmethyl
DPMS	diphenylmethylsilyl

Dpp	diphenylphosphinyl
DPP-Cl	diphenylphosphinyl chloride
DPPA	diphenylphosphoryl azide
DPPC	dipalmitoylphosphatidylcholine
Dppe	2-(diphenylphosphino)ethyl
Dppm	diphenyl-4-pyridylmethyl
DPS	*trans-p,p′*-diphenylstilbene
DiPT	diisopropyl tartrate
DSAH	disuccinimidyl (*N,N′*-diacetyl-homocysteine)
DSP	dithiobis(succinimidyl propionate)
DSS	3-(trimethylsilyl)-1-propane-sulfonic acid (sodium salt)
DSS	disuccinimidyl suberate
DSS	2,2-dimethyl-2-silapentane-5-sulfonate
DST	disuccinimidyl tartrate
DTBMS	di-*tert*-butylmethylsilyl
DTBS	di-*tert*-butylsilylene
DTE	dithioerythritol
DTMC	4,4′-dichloro-α-(trichloromethyl)-benzhydrol
DTNB	5,5′-dithiobis(2-nitrobenzoic acid)
DTPA	diethylenetriaminepentaacetic acid
Dts	dithiasuccinimidyl
DTT	dithiothreitol
DVB	divinylbenzene
DXE	dixylylethane
EAA	ethyl acetoacetate
EAA	*N*-ethylanthranilic acid
EADC	ethylaluminium dichloride
EAK	ethyl amyl ketone
EASC	ethylaluminium sesquichloride
EBA	*N*-ethyl-*N*-benzylaniline
EBASA	*N*-ethyl-*N*-benzylaniline-4-sulfonic acid
EBSA	*p*-ethylbenzenesulfonic acid
ECEA	*N*-ethyl-*N*-chloroethylaniline
EDANS	2-aminoethylamino-1-naphthalene-sulfonic acid (1,5 or 1,8)
EDB	ethylene dibromide
EDC	ethylene dichloride
EDCI	1-ethyl-3-[3-(dimethylamino)-propyl]carbodiimide hydro-chloride
EDDP	*O*-ethyl *S,S*-diphenyl dithio-phosphate
EDTA	ethylenediaminetetraacetic acid
EDTN	1-ethoxy-4-(dichloro-*s*-triazinyl)-naphthalene
EDTP	ethylenediamine tetrapropanol
EE	1-ethoxyethyl
EEDQ	*N*-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline
EGS	ethylene glycol bis(succinimidyl succinate)
EGTA	1,2-bis(2-aminoethoxy)ethane-*N,N,N′,N′*-tetraacetic acid
en	ethylenediamine
EPN	*O*-ethyl *O*-(*p*-nitrophenyl)-thiobenzenephosphate
EPPS	4-(2-hydroxyethyl)-1-piperazine-propanesulfonic acid
Et	ethyl
ETA	(see EDTA)
ETSA	ethyl trimethylsilylacetate
EVK	ethyl vinyl ketone
FA	furfuryl alcohol
FAD	flavin adenine dinucleotide
FAMSO	methyl methylsulfinylmethyl sulfide
Fc	ferrocenyl
FDMA	perfluoro-*N,N*-dimethylcyclohexyl-methylamine
FDNB	(see DNF)
FDNDEA	5-fluoro-2,4-dinitro-*N,N*-diethyl-aniline
FDP	D-fructose-1,6-diphosphate
FHZ	ferritin hydrazide
FITC	fluorescein isothiocyanate
Fl	flavin
Fm	9-fluorenylmethyl
FMA	fluorescein mercuric acetate
FMN	flavin mononucleotide
Fmoc	9-fluorenylmethoxycarbonyl
FNPS	bis(4-fluoro-3-nitrophenyl) sulfone
For	formyl
FS	Fremy's salt (dipotassium nitroso-disulfonate)
FTN	perfluoro-1,3,7-trimethylbicyclo-[3.3.1]nonane
FUDR	5-fluorodeoxyuridine
G	guanine
GABA	4-aminobutyric acid
GAPDH	glyceraldehyde-3-phosphate dehydrogenase
GDP	guanosine 5′-diphosphate
GLDH	glutamate dehydrogenase
Gln	glutamine

Glu	glutamic acid
Gly	glycine
Glyme (glyme)	1,2-dimethoxyethane (see DME)
GLYMO	3-glycidyloxypropyl-trimethoxysilane
GMP	guanosine 5′-monophosphate
GOD	glucose oxidase
G-6-P	glucose-6-phosphate
GSH	glutathione, reduced
GSSG	glutathione, oxidized hydrate
GTP	guanosine 5′-triphosphate
GUM	guaiacolmethyl
HABA	2-(*p*-hydroxyphenylazo)benzoic acid
HABBA	2-(4′-hydroxyazobenzene)benzoic acid
Hb	haemoglobin
HBD	hexabutyldistannoxane
HDCBS	2-hydroxy-3,5-dichlorobenzene-sulfonic acid
HDODA	1,6-hexanediol diacrylate
HDPE	high-density polyethylene
HEA	*N*-(2-hydroxyethyl)aziridine
HEDTA	2-hydroxyethylethylenediamine-triacetic acid
HEEI	*N*-(2-hydroxyethyl)ethyleneimine
HEMA	2-hydroxyethyl methacrylate
HEPES	4-(2-hydroxyethyl)-1-piperazine-ethanesulfonic acid
HEPSO	N-hydroxyethylpiperazine-*N*′-2-hydroxypropanesulfinic acid
HETE	hydroxy(e)icosatetraenoic acid
Hex	hexane (or hexyl)
HFA	hexafluoroacetone
HFBA	heptafluorobutyric acid
HFIP	hexafluoroisopropyl alcohol
HFP	hexafluoropropene
HFTA	hexafluorothioacetone
HHPA	hexahydrophthalic anhydride
His	histidine
HMAT	hexa[1-(2-methyl)aziridinyl]-1,3,5-triphosphatriazine
HMB	2-hydroxy-4-methoxybenzo-phenone
HMB	2-hydroxy-5-methoxybenzaldehyde
HMDS	1,1,1,3,3,3-hexamethyldisilazane
HMDSO	hexamethyldisiloxane
HMI	hexamethyleneimine
HMN	2,2,4,4,6,8,8-heptamethylnonane
HMPA	hexamethylphosphoramide (hexamethylphosphoric triamide)
HMPT	hexamethylphosphorous triamide
HMPTA	(see HMPA)
HMTT	3-hexadecanoyl-4-methoxy-carbonyl-1,3-thiazolidine-2-thione
HOAc	acetic acid
HOBT	1-hydroxybenzotriazole
HONB	*N*-hydroxy-5-norbornene-2,3-dicarboxylic acid imide
HOSA	hydroxylamine-*O*-sulfonic acid
HPETE	hydroperoxy(e)icosatetraenoic acid
HPPH	5-hydroxyphenyl-5-phenyl-hydantoin
HQ	hydroquinone
HTMP	4-hydroxy-2,2,6,6-tetramethyl-piperidine
HVA	homovanillic acid (4-hydroxy-3-methoxyphenylacetic acid)
Hyiv	α-hydroxyisovaleric acid
Hz	homobenzyloxycarbonyl
I-AEDANS	*N*-iodoacetyl-*N*′-(*X*-sulfo-1-naphthyl)ethylenediamine (*X* = 5, 1,5-I-AEDANS; *X* = 8, 1,8-I-AEDANS)
IBD	iodobenzene dichloride
IBMX	3-isobutyl-1-methylxanthine
IBTMO	isobutyltrimethoxysilane
ICD	isocitric dehydrogenase
ICl	isophthaloyl chloride
IDP	inosine 5′-diphosphate
IDTr	3-(imidazol-1-ylmethyl)-4,4′-di-methoxytriphenylmethyl
IDU	5-iodo-2′-deoxyuridine
IH	immobilized histamine
IIDQ	2-isobutoxy-1-isobutoxycarbonyl-1,2-dihydroquinoline
Ile	isoleucine
Im	1-imidazolyl
IMds	2,6-dimethoxy-4-methylbenzene-sulfonyl
IMEO	imidazolinepropyltriethoxysilane
IMP	inosine 5′-monophosphate
INAH	isonicotinic acid hydrazide
INH	(see INAH)
INT	2-(*p*-iodophenyl)-3-(*p*-nitro-phenyl)-5-phenyltetrazolium chloride
IPA	isopropyl alcohol

Ipaoc	1-isopropylallyloxycarbonyl
IPC	isopropyl *N*-phenylcarbamate
$IpcBH_2$	isopinocampheylborane
Ipc_2BH	diisopinocampheylborane
IPDI	isophorone diisocyanate (3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate)
IPDMS	isopropyldimethylsilyl
IPN	isophthalonitrile
IPOTMS	isopropenyloxytrimethylsilane
Ips	[(4-iodophenyl)sulfonyl]
IPTG	isopropyl β-D-thiogalactoside
ITA	itaconic anhydride
ITP	inosine 5′-triphosphate
IZAA	5-chloroindazol-3-acetic acid ethyl ester
KAPA	potassium 3-aminopropylamide
KBA	3-ketobutyraldehyde dimethyl acetal
KBT	4-ketobenztriazine
KDO	2-keto-3-deoxyoctonate
K-Selectride®	potassium tri-*sec*-butylborohydride
KS-Selectride®	potassium trisiamylborohydride
LAH	lithium aluminium hydride
LAP	leucine aminopeptidase
LDA	lithium diisopropylamide
LDBB	lithium 4,4′-di-*tert*-butylbiphenylide
LDH	lactic dehydrogenase
LDPE	low-density polyethylene
Leu	leucine
Lev	levulinoyl
LevS	[4,4-(ethylenedithio)pentanoyl]
Lgf_2BH	dilongifolylborane
LHMDS	lithium hexamethyldisilazane
LICA	lithium isopropylcyclohexylamide
LPO	lauroyl peroxide
L-Selectride®	lithium tri-*sec*-butylborohydride
LS-Selectride®	lithium trisiamylborohydride
LT	leukotriene
LTA	lead tetraacetate
LTMAC	dodecyltrimethylammonium chloride
LTMP	lithium 2,2,6,6-tetramethylpiperidide
Lys	lysine
M	metal
MA	maleic anhydride
MAA	menthoxyacetic acid
MAA	methyl acetoacetate
MABR	methylaluminium bis(4-bromo-2,6-di-*tert*-butylphenoxide)
MAD	methylaluminium bis(2,6-di-*tert*-butyl-4-methylphenoxide)
Mal	maleyl
-Mal-	maleoyl
Mal<	maleoyl
MAM-acetate	methylazoxymethyl acetate
MAPO	tris[1-(2-methyl)aziridinyl]-phosphine
Phenyl-MAPO	bis[1-(2-methyl)aziridinyl]phenylphosphine oxide
MAPS	tris[1-(2-methyl)aziridinyl]-phosphine sulfide
MAPTAC	methacrylamidopropyltrimethylammonium chloride
MASC	methylaluminium sesquichloride
MBA	*N*,*N*′-methylenebisacrylamide
MBBA	*N*-(*p*-methoxybenzylidene)-*p*-butylaniline
MBE	1-methyl-1-benzyloxyethyl
MBF	2,3,3*a*,4,5,6,7,7*a*-octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl
MBS	*m*-maleimidobenzoyl-*N*-hydroxysuccinimide ester
MBS	*p*-methoxybenzenesulfonyl
MBTH	3-methyl-2-benzothiazolinone hydrazone
MC	magnesium chlorate
3-MC	3-methylcholanthrene
MCA	monochloroacetic acid
MCAA	(see MCA)
3,3-MCH	3-methyl-3-cyclohexen-1-one
MCP	*meta*-cresol purple (*m*-cresol purple)
MCP	methylcyclopentane
MCPBA	*m*-chloroperoxybenzoic acid
MCPCA	2-methyl-4-chlorophenoxyaceto-*o*-chloroanilide
MCPDEA	*N*,*N*-di(2-hydroxyethyl)-*m*-chloroaniline
MCPP	4-chloro-3-methylphenoxypropionic acid
MDA	1,8-*p*-menthanediamine
MDEB	*N*-methyl-*N*-dodecylephedrinium bromide
MDH	malic dehydrogenase

Mds	2,6-dimethyl-4-methoxybenzene-sulfonyl
Me	methyl
MeCCNU	1-(2-chloroethyl)-3-(4-*trans*-methylcyclohexyl)-1-nitrosourea
MEI	2-morpholinoethyl isocyanide
MEK	methyl ethyl ketone
MeLeu	*N*-methylleucine
MEM	2-methoxyethoxymethyl
MEMCl	2-methoxyethoxymethyl chloride
MEMO	3-methacryloxypropyltrimethoxy-silane
1-MEO-PMS	1-methoxy-5-methylphenazinium methyl sulfate
MeOZ	*p*-methoxybenzyloxycarbonyl
MEP	*O*,*O*-dimethyl *O*-(3-methyl-4-nitro-phenyl) phosphorothioate
Mes	mesityl
MES·hydrate	4-morpholineethanesulfonic acid
Met	methionine
Meth	2-mercaptoethanol
MG-Ch	methyl glycol chitosan
MHHPA	4-methylhexahydrophthalic anhydride
MIA	*N*-methylisatoic anhydride
MIBK	methyl isobutyl ketone
MICA	magnesium isopropyl cyclo-hexamide
MIPK	methyl isopropyl ketone
MIX	3-isobutyl-1-methylxanthine
MMA	methyl methacrylate
MMAA	mono-*N*-methylacetoacetamide
MMC	methyl magnesium carbonate
MMH	methyl mercuric hydroxide
MMS	methyl methanesulfonate
MMTrCl	monomethoxytrityl chloride
MMTS	(see FAMSO)
MNA	methylnadic anhydride (methyl-norbornene-2,3-dicarboxylic acid anhydride)
MNNG	*N*-methyl-*N*′-nitro-*N*-nitroso-guanidine
MNPT	*m*-nitro-*p*-toluidine
MO	methyl orange
MOM	methoxymethyl
MoOPH	oxodiperoxymolybdenum-(pyridine) hexamethyl-phosphoramide
MOPS	4-morpholinepropanesulfonic acid
MOPSO	3-(*N*-morpholino)-2-hydroxy-propanesulfonic acid
Moz	*p*-methoxybenzyloxycarbonyl
6MP	6-mercaptopurine
MPEMA	2-ethyl-2-(*p*-tolyl)malonamide
MPM	(*p*-methoxyphenyl)methyl
MPP	*O*,*O*-dimethyl *O*-(4-methyl-mercapto-3-methylphenyl) thiophosphate
MPPH	5-(*p*-methylphenyl)-5-phenyl-hydantoin
MPS	methyl phenyl sulfide
Mps	*p*-methoxyphenylsulfonyl
Mpt	dimethylthiophosphinyl
Mpt-Cl	methylphosphinothionyl chloride
MR	methyl red
MRITC	methylrhodamine isothiocyanate
MS (or Ms)	mesyl (or methanesulfonyl)
MSA	methanesulfonic acid
MsCl	methanesulfonyl chloride
MSH	2,4,6-trimethylbenzenesulfonyl hydrazide
Msib	4-(methylsulfinyl)benzyl
MSMA	monosodium methanearsonate
MSO	*p*-cresyl methyl ether
MSOC	*N*-(2-methylsulfonyl)ethyloxy-carbonyl
MST	mesitylenesulfonyltetrazolide
MSTFA	*N*-methyl-*N*-trimethylsilyl-trifluoroacetamide
Msz	4-methylsulfonylbenzyloxy-carbonyl
α-MT	DL-α-methyltyrosine
MTB	methylthymol blue
Mtb	2,4,6-trimethoxybenzenesulfonyl
MTBE	*tert*-butyl methyl ether
MTBSTFA	*N*-(*tert*-butyldimethylsilyl)-*N*-methyltrifluoroacetamide
MTC	methyl isothiocyanate
MTCA	2-methylthiazolidine-4-carboxylic acid
MTD	*m*-toluenediamine
MTDEA	*N*,*N*-di(2-hydroxyethyl)-*m*-toluidine (*m*-toluidine-*N*,*N*-diethanol)
Mte	2,3,5,6-tetramethyl-4-methoxy-benzenesulfonyl
MTES	methyltriethoxysilane
MTG	methyl β-D-thiogalactoside
MTH	methylthiohydantoin
MTHP	4-methoxytetrahydropyranyl
MTHPA	methyltetrahydrophthalic anhydride
MTM	methylthiomethyl

MTMB	4-(methylthiomethoxyl)butanoyl
MTMC	4-(methylthio)-*m*-cresol
MTMECO	2-(methylthiomethoxy)-ethoxycarbonyl
MTMS	methyltrimethoxysilane
MTMT	2-(methylthiomethoxymethyl)-benzoyl
MTN	*m*-tolunitrile
MTP	4-(methylthio)phenol
MTPA	α-methoxy-α-trifluoromethyl-phenylacetic acid
Mtpc	4-methylthiophenoxycarbonyl
Mtr	2,3,6-trimethyl-4-methoxy-benzenesulfonyl
Mts	2,4,6-trimethylbenzenesulfonyl
MTT	3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2*H*-tetrazolium bromide
MTX	(+)-amethopterin
MUGB	4-methylumbelliferyl *p*-guanidinobenzoate
MVK	methyl vinyl ketone
MVP	2-methyl-5-vinylpyridine
MXDA	*m*-xylylenediamine
5-NAA	5-nitroanthranilic acid
NAAD	nicotinic acid adenine dinucleotide
NAC	1-naphthyl *N*-methylcarbamate
NAD	nicotinamide adenine dinucleotide
NADH	nicotinamide adenine dinucleotide phosphate, reduced
NAI	*N*-acetylimidazole
NAM	*N*-acetylmethionine
NANA	*N*-acetylneuraminic acid
NAP	4-nitroaminophenol
NB	*p*-nitrobenzyl
NBA	*N*-bromoacetamide
NBDCl	4-chloro-7-nitro-2,1,3-benzoxadiazole
NBD-F	7-fluoro-4-nitro-2,1,3-diazole
NBMPR	*S*-(*p*-nitrobenzyl)-6-thioinosine
NBS	*N*-bromosuccinimide
Nbs	[(3-carboxy-4-nitrophenyl)thio]
NBSac	*N*-bromosaccharin
NBSC	2-nitrobenzenesulfenyl chloride
NCA	*N*-chloroacetamide
NCDC	2-nitro-4-carboxyphenyl *N*,*N*-diphenylcarbamate
NCN	cyanonaphthalene
NCS	*N*-chlorosuccinimide
NEM	*N*-ethylmaleimide
NEP	*N*-ethyl-2-pyrrolidinone
NEPIS	*N*-ethyl-5-phenylisoxazolium-3′-sulfonate
NesMIC	(+)-(neomenthylsulfonyl)methyl isocyanide
5-NIA	5-nitroisatoic anhydride
NIP	4-hydroxy-5-nitro-3-iodophenyl-acetic acid
NIP	2,4-dichlorophenyl 4′-nitrophenyl ether
NIS	*N*-iodosuccinimide
NM	nitromethane
NMA	*N*-methylolacrylamide
NMO	*N*-methylmorpholine *N*-oxide
NMP	*N*-methylphthalimide
NMP	*N*-methyl-2-pyrrolidone
NMSO	4-methyl-2-nitroanisole
Noc	4-nitrocinnamyloxycarbonyl
NP-	*p*-nitrophenyl
p-NPDPP	*p*-nitrophenyl diphenyl phosphate
α-NPO	2-(1-naphthyl)-5-phenyloxazole
NPP	2-nitro-2-propenyl pivalate
NPS	*o*-nitrophenylsulfenyl
NPSP	*N*-phenylselenenylphthalimide
Npys-Cl	3-nitro-2-pyridinesulfenyl chloride
N-Selectride®	sodium tri-*sec*-butylborohydride
NTA	nitrilotriacetic acid
N-t-B	2-methyl-2-nitrosopropane
Nu	nucleophile
OCAD	*o*-chlorobenzaldehyde
OCBA	*o*-chlorobenzoic acid
OCBC	*o*-chlorobenzyl chloride
OCBN	*o*-chlorobenzonitrile
OCCN	*o*-chlorobenzyl cyanide
OCDC	*o*-chlorodichlorotoluene
OCOC	*o*-chlorobenzoyl chloride
OCPA	*o*-chlorophenylacetic acid
OCPT	2-chloro-4-aminotoluene (*o*-chloro-*p*-aminotoluene)
OCT	*o*-chlorotoluene
OCT	ornithine carbamyl transferase
OCTC	*o*-chlorobenzotrichloride
OCTEO	octyltriethoxysilane
ODA	4,4′-oxydianiline
OMH-1	sodium diethyldihydroaluminate
OMP	orotidine 5′-monophosphate
ONB	*o*-nitrobenzyl
OTB	*o*-toluidine boric acid
OTD	*o*-toluenediamine

P	polymer substituent
PABA	*p*-aminobenzoic acid
PADA	poly(adipic anhydride)
PADA	pyridine-2-azo-*p*-dimethylaniline
Bromo-PADAP	2-(5-bromo-2-pyridylazo)-5-diethylaminophenol
PAH	polycyclic aromatic hydrocarbon
PAH	*p*-aminohippuric acid
PAL	phenylalanine ammonia lyase
PAM	pyridine-2-aldoxime methiodide
2-PAM	(see PAM)
2-PAMCl	2-pyridinealdoxime methochloride
PAN	1-(2-pyridylazo)-2-naphthol
PAP	*O,O*-dimethyl *S*-α-(ethoxycarbonyl)benzyl phosphorothiolothioate
PAPA	poly(azelaic anhydride)
PAPS	3′-phosphoadenosine-5′-phosphosulfate
PAR	4-(2-pyridylazo)resorcinol, sodium salt monohydrate
PAS	*p*-aminosalicylic acid
PASAM	*p*-toluenesulfonamide
PBA	*p*-benzoquinone-2,3-dicarboxylic anhydride
PBBO	2-(4-biphenylyl)-6-phenylbenzoxazole
PBD	2-(4-biphenylyl)-5-phenyl-1,3,4-oxadiazole
Butyl-PBD	2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)1,3,4-oxadiazole
PBI	*p*-benzoquinone-2,3-dicarboxylic imide
PBN	*N*-*tert*-butyl-α-phenylnitrone
PBP	*p*-(benzyloxy)phenol
PBS	poly(butene-1-sulfone)
PBz	*p*-phenylbenzoyl
PC	propylene carbonate
PCAD	*p*-chlorobenzaldehyde
PCB	polychlorobiphenyl
PCBA	*p*-chlorobenzoic acid
PCBC	*p*-chlorobenzyl chloride
PCBN	*p*-chlorobenzonitrile
PCBTF	*p*-chlorobenzotrifluoride
PCC	pyridinium chlorochromate
PCCN	*p*-chlorobenzyl cyanide
PCDC	*p*-chlorodichlorotoluene
P-Cellulose	cellulose phosphate
PCMB	*p*-chloromercuribenzoic acid
PCMX	*p*-chloro-*m*-xylenol
PCNB	pentachloronitrobenzene
PCOC	*p*-chlorobenzoyl chloride
PCONA	*p*-chloro-*o*-nitroaniline
PCOT	4-chloro-2-aminotoluene (*p*-chloro-*o*-aminotoluene)
PCP	pentachlorophenol
PCPA	*p*-chlorophenylacetic acid
PCT	polychloroterphenyl
PCT	*p*-chlorotoluene
PCTC	*p*-chlorobenzotrichloride
PDA	phorbol 12,13-diacetate
PDBz	phorbol 12,13-dibenzoate
PDC	pyridinium dichromate
PDEA	*N*-phenyldiethanolamine
PDQ	sodium (2-methyl-4-chlorophenoxy)butyrate
PDT	3-(2-pyridyl)-5,6-diphenyl-1,2,4-triazine
PEA	*N*-(2-hydroxyethyl)aniline (*N*-phenylethanolamine)
PEEA	*N*-(2-hydroxyethyl)-*N*-ethylaniline (*N*-phenyl-*N*-ethylethanolamine)
PEEK	poly(ether ether ketone)
PEG	poly(ethylene glycol)
PEI-cellulose	polyethyleneimine-impregnated cellulose
PEMA	2-ethyl-2-phenylmalonamide
Peoc	2-phosphonioethoxycarbonyl
Peoc	2-(triphenylphosphonio)-ethoxycarbonyl
PEP	phosphoenolpyruvic acid
Pet	2-(2-pyridyl)ethyl
PET	poly(ethylene terephthalate)
PETA	pentaerythritol triacrylate
PG	protective group
PG	prostaglandin
PGE	phenyl glycidyl ether
Ph	phenyl
Phe	phenylalanine
Phenoc	4-methoxyphenacyloxycarbonyl
PHR	phorbol
Pht	phthalyl
Phth	phthaloyl
PIA	phenyliodoso diacetate
PIPES	1,4-piperazinebis(ethanesulfonic acid)
Pixyl	9-phenylxanthenyl
PMA	phorbol 12-myristate 13-acetate
PMA	phenylmercuric acetate
PMB	*p*-methoxybenzyl
PMBM	*p*-methoxybenzyloxymethyl

Pmc	2,2,5,7,8-pentamethylchroman-6-sulfonyl
PMDTA	pentamethyldiethylenetriamine
Pme	pentamethylbenzenesulfonyl
PMEA	*N*-(2-hydroxyethyl)-*N*-methylaniline (*N*-phenyl-*N*-methylethanolamine)
PMH	phenylmercuric hydroxide
PMHS	polymethylhydrosiloxane
PMI	3-phenyl-5-methylisoxazole
PMI-ACID	3-phenyl-5-methylisoxazole-4-carboxylic acid
PMP	*O*,*O*-dimethyl *S*-(phthalimidomethyl) phosphorodithioate
PMP	1,2,2,6,6-pentamethylpiperidine
PMS	phenazine methosulfate
PMS	*p*-methylbenzylsulfonyl
PNASA	*p*-nitroaniline-*o*-sulfonic acid
PNMT	phenylethanolamine-*N*-methyltransferase
PNOT	*p*-nitro-*o*-toluidine
PNPDPP	*p*-nitrophenyl diphenyl phosphate
PNPG	α-*p*-nitrophenylglycerine
PNPP	*p*-nitrophenyl phosphate
POBN	α-(4-pyridyl-1-oxide)-*N*-*tert*-butylnitrone
4-POBN	(see POBN)
POC	cyclopentyloxycarbonyl
POM	chloromethyl pivalate
POM	4-pentenyloxymethyl
POM	pivaloyloxymethyl
POPOP	1,4-bis(5-phenyloxazol-2-yl)-benzene
Dimethyl-POPOP	1,4-bis(4-methyl-5-phenyloxazol-2-yl)benzene
POPSO	piperazine-*N*,*N*′-bis(2-hydroxypropanesulfonic acid)
PPA	polyphosphoric acid
PPDA	phenyl phosphorodiamidate
PPDP	*p*,*p*′-diphenol
PPE	polyphosphate ester (ethyl *m*-phosphate)
PPNCl	bis(triphenylphosphoranylidene)-ammonium chloride
PPO	2,5-diphenyloxazole
Ppoc	2-triphenylphosphonioisopropoxycarbonyl
Ppt	diphenylthiophosphinyl
PPTS	pyridinium *p*-toluenesulfonate
Pr	propyl
PR	phenol red
iPr	isopropyl
Pro	proline
P2S	2-pyridinealdoxime methyl methanesulfonate
PS-Cl	2-pyridinesulfenyl chloride
Psec	2-(phenylsulfonyl)ethoxycarbonyl
PSPA	poly(sebacic anhydride)
PTAD	*N*-phenyl-1,2,4-triazoline-3,5-dione
PTAP	phenyltrimethylammonium perbromide
PTBBA	*p*-*tert*-butylbenzoic acid
Ptc	phenyl(thiocarbamoyl)
PTC	phenyl isothiocyanate
PTH	phenylthiohydantoin
PTM	phenylthiomethyl
PTMO	n-propyltrimethoxysilane
PTSA	*p*-toluenesulfonic acid
PTSI	*p*-toluenesulfonyl isocyanate
Pv	pivaloyl
PVA	poly(vinyl alcohol)
PVC	poly(vinyl chloride)
PVDF	poly(vinylidene fluoride)
PVP	polyvinylpyrrolidone
PVPDC	poly(4-vinylpyridinium) dichromate
PVP-I	polyvinylpyrrolidone–iodine complex
PVSK	potassium poly(vinyl sulfate)
Pyoc	2-(pyridyl)ethoxycarbonyl
PyOTs	(see PPTS)
Pyr (or Py)	pyridine
Pz	4-phenylazobenzoyloxycarbonyl
Qu	8-quinolinyl
QUIBEC	benzylquinidinium chloride
RAMP	(*R*)-1-amino-2-(methoxymethyl)-pyrrolidine
RDB	sodium dihydrobis(2-methoxyethoxy)aluminate
Red-Al®	(see RDB)
RNA	ribonucleic acid
RNase	ribonuclease
SAA	succinic anhydride
SADP	*N*-succinimidyl (4-azidophenyldithio)propionate
SAMP	(*S*)-1-amino-2-(methoxymethyl)-pyrrolidine
SBH	sodium borohydride
Scm	*S*-carboxymethylsulfenyl

SDP	4,4′-sulfonyldiphenol
SDPP	*N*-succinimidyl diphenyl phosphate
SDS	sodium dodecyl sulfate
SDS	sodium dodecylbenzenesulfonate
SEM	2-(trimethylsilyl)ethoxymethyl
Ser	serine
SES	2-(trimethylsilyl)ethanesulfenyl
SEX	sodium ethyl xanthate
Sia_2BH	disiamylborane
SLS	sodium lauryl sulfate
SMCC	succinimidyl 4-(*N*-maleimido-methylcyclohexane)-1-carboxylate
SMOM	(phenyldimethylsilyl)ethoxymethyl
SMPB	succinimidyl 4-(*p*-maleimido-phenyl)butyrate
Di-SNADNS	2,7-bis(4-sulfo-1-naphthylazo)-1,8-dihydroxynaphthalene-3,6-disulfonic acid
Snm	*S*-(*N*-methyl-*N*-phenyl-carbamoyl)sulfenyl
SPA	superphosphoric acid
SPADNS	2-(*p*-sulfophenylazo)-1,8-dihydroxy-3,6-naphthalene-disulfonic acid (trisodium salt)
SPDP	*N*-succinimidyl 3-(2-pyridyldithio)-propionate
SSP	1,2-distearoylpalmitin
STABACE	1,1,4,4-tetramethyldisilyl-azacyclopentane
STPP	sodium tripolyphosphate
Su	succinimido
Suc	3-carboxypropanoyl
-Suc-	succinyl
Super-Hydride®	lithium triethylborohydride
2,4,5-T	2,4,5-trichlorophenoxyacetic acid
TAC	triallyl cyanurate
Tacm	trimethylacetamidomethyl
TAMA	*N*-methylanilinium trifluoroacetate
TAME	*N*-α-*p*-tosyl-L-arginine methyl ester hydrochloride
TAMM	tetrakis(acetoxymercuri)methane
TAPA	α-(2,4,5,7-tetranitro-9-fluor-enylideneaminooxy)propionic acid
TAPS	3-[tris(hydroxymethyl)methyl-amino]-1-propanesulfonic acid
TAPSO	3-[*N*-(tris(hydroxymethyl)methyl-amino]2-hydroxypropane-sulfonic acid
TAS	tris(diethylamino)sulfonium
TASF	tris(dimethylamino)sulfonium (trimethylsilyl)difluoride
TB	thexylborane
TB	thymol blue
2,3,6-TBA	2,3,6-trichlorobenzoic acid
TBAB	tetrabutylammonium bromide
TBAC	*tert*-butylacetyl chloride
TBAF	tetrabutylammonium fluoride
TBAF	tetra-n-butylammonium fluoroborate
TBAHS	tetrabutylammonium hydrogen sulfate
TBAP	tetra-n-butylammonium perchlorate
TBAS	tetra-n-butylammonium succinimide
TBC	*p-tert*-butylcatechol
TBDA	thexylborane-*N*,*N*-diethylaniline
TBDMS	(see TBS)
TBDMSCl	(see TBSCl)
TBDMSI	1-(*tert*-butyldimethylsilyl)-imidazole
TBDPS	*tert*-butyldiphenylsilyl
TBDS	tetra-*tert*-butoxydisilane-1,3-diylidene
TBE	1,1,2,2-tetrabromoethane
TBHC	*tert*-butyl hypochlorite
TBHP	*tert*-butyl hydroperoxide
TBMPS	*tert*-butylmethoxyphenylsilyl
TBO	3-[(trimethylsilyl)oxy]-3-buten-2-one
TBP	tri-n-butyl phosphate
TBP	triphenylbutylphosphonium bromide
TBS	*tert*-butyldimethylsilyl
TBSCl	*tert*-butyldimethylsilyl chloride
TBTD	tetrabutylthiuram disulfide
TBTr	4,4′,4″-tris(benzyloxy)-triphenylmethyl
TBUP	tri-n-butylphosphine
TC	2,3,4,5-tetraphenylcyclo-pentadienone
TCA	trichloroacetic acid
TCB	trichlorobenzene (usually 1,3,5)
TcBoc	1,1-dimethyl-2,2,2-trichloro-ethoxycarbonyl
Tce	2,2,2-trichloroethyl
Tcec	β,β,β-trichloroethoxycarbonyl
TcecCl	β,β,β-trichloroethoxycarbonyl chloride

TCl	terephthaloyl chloride
TCNE	tetracyanoethylene
TCNP	11,11,12,12-tetracyanopyreno-2,7-quinodimethane
TCNQ	7,7,8,8-tetracyanoquinodimethane
TCP	tricresyl phosphate
TCP	trichlorophenol (usually 2,4,5 or 2,4,6)
Tcp	2,4,5-trichlorophenyl
Tcroc	2-(trifluoromethyl)-6-chromonyl-methylenecarbonyl
Tcrom	2-(trifluoromethyl)-6-chromonyl-methylene
TCTFP	1,1,2,2-tetrachloro-3,3,4,4-tetra-fluorocyclobutane
TDI	tolylene diisocyanate
TDP	4,4′-thiodiphenol
TDS	thexyldimethylsilyl
TEA	triethanolamine
TEA	triethylaluminium
TEA	triethylamine
TEAB	triethylammonium bicarbonate
TEAE-cellulose	triethylaminoethyl cellulose
TEAS	tetraethylammonium succinimide
TEBA or TEBAC	benzyltriethylammonium chloride
TED	(see DABCO)
TEG	triethylene glycol
TEM	triethylenediamine (1,4-diaza-bicyclo[2.2.2]octane)
TEMPO	2,2,6,6-tetramethylpiperidinooxy, free radical
Teoc	2-trimethylsilylethoxycarbonyl
TES	triethylsilyl
TES	2-[tris(hydroxymethyl)methyl-amino]-1-ethanesulfonic acid
TES	*N*,*N*,*N*′,*N*′-tetraethylsulfamide
TETD	tetraethylthiuram disulfide
TETM	tetraethylthiuram monosulfide
TETN	triethylamine
Tf	trifluoromethanesulfonyl
TFA	trifluoroacetic acid
TFA	trifluoroacetyl
TFAA	trifluoroacetic anhydride
TFA-ME	methyl trifluoroacetate
TFE	2,2,2-trifluoroethanol
TFMC-Eu	tris[3-(trifluoromethylhydroxy-methylene)-*d*-camphorato]·Eu(III)
TFMC-Pr	tris[3-(trifluoromethylhydroxy-methylene)-*d*-camphorato]·Pr(III)
THAM	tris(hydroxymethyl)aminomethane
THE	tetrahydrocortisone
THF	tetrahydrofuran, tetrahydrofuranyl
THF	tetrahydrofolic acid
THFA	tetrahydrofurfuryl alcohol
THFC-Eu	tris[3-(heptafluoropropylhydroxy-methylene)-*d*-camphorato]·Eu(III)
THIP	4,5,6,7-tetrahydroisoxazolo[5,4-*c*]-pyrimidin-3(2*H*)-one
THP	tetrahydropyran (or tetra-hydropyranyl)
Thr	threonine
Thx	thexyl (2,3-dimethyl-2-butyl)
TIBA	triiodobenzoic acid (usually 2,3,5)
TIBA	triisobutylaluminium
TIPDS	1,3-(1,1,3,3-tetraisopropyl-disilanoxylidene)
TIPS	triisopropylsilyl
TIPSCl	1,3-dichloro-1,1,3,3-tetra-isopropyldisiloxane
TLCK	1-chloro-3-tosylamido-7-amino-2-heptanone hydrochloride
TLTr	4,4′,4″-tris(levulinoyloxy)-triphenylmethyl
TMA	trimethylaluminium
TMAC	trimellitic anhydride monoacid chloride
TMAEMC	2-trimethylammoniumethyl-methacrylic chloride
TMAT	tetramethylammonium tribromide
TMAT	tris-2,4,6-[1-(2-methyl)aziridinyl]-1,3,5-triazine
TMB	3,3′,5,5′-tetramethylbenzidine
TMB	*N*,*N*,*N*′,*N*′-tetramethylbenzidine
TMB-4	1,1′-trimethylenebis[4-(hydroxy-iminomethyl)pyridinium bromide]
TMBA	3,4,5-trimethylbenzaldehyde
TMC	3,3,5-trimethylcyclohexanol
TMCS	(see TMSCl)
TMEDA	*N*,*N*,*N*′,*N*′-tetramethylethylene-diamine
TMG	methyl β-D-thiogalactoside
TMM	trimethylenemethane
TMO	trimethylamine *N*-oxide
TMP	2,2,6,6-tetramethylpiperidine
TMP	thymidine 5′-monophosphate

TMPM	trimethoxyphenylmethyl
TMPTA	trimethylolpropane triacrylate
TMPTMA	trimethylolpropane trimethacrylate
TMS	trimethylsilyl
TMS	tetramethylsilane
TMSCl	trimethylsilyl chloride
TMSCN	trimethylsilyl cyanide
TMSDEA	*N*,*N*-diethyl-1,1,1-trimethylsilylamine
TMSEC	2-(trimethylsilyl)ethoxycarbonyl
TMTD	tetramethylthiuram disulfide
TMTM	tetramethylthiuram monosulfide
TMTr	tris(*p*-methoxyphenyl)methyl
TNBA	tri-n-butylaluminium
TNBT	tetranitro blue tetrazolium
TNF	2,4,7-trinitrofluorenone
TNM	tetranitromethane
TNPA	tri-n-propylaluminium
TNS	6-(*p*-toluidino)-2-naphthalenesulfonic acid, potassium salt
TNT	2,4,6-trinitrotoluene
Tol	toluene or *p*-tolyl
TOPO	tri-n-octylphosphine oxide
TOS	*p*-toluenesulfonyl (tosyl)
TosMIC	tosylmethyl isocyanide
TP	thymolphthalein
TPB	1,1,4,4-tetraphenyl-1,3-butadiene
TPC	thymolphthalein complexone
TPCD	tetraphenylcyclopentadienone
TPCK	L-1-*p*-tosylamino-2-phenylethyl chloromethyl ketone
TPE	tetraphenylethylene
TPN	triphosphopyridine nucleotide, sodium salt
TPNH	reduced triphosphopyridine nucleotide, sodium salt
TPP	tetraphenylporphyrin
TPP	triphenyl phosphate
TPP	triphenylphosphine
TPS	2,4,6-triisopropylbenzenesulfonyl
TPS	triphenylsilyl
TPS	triphenylsulfonium chloride
TPSCl (or TPS)	2,4,6-triisopropylbenzenesulfonyl chloride
TPTZ	2,4,6-tris(2-pyridyl)-*s*-triazine
TRIAMO	triaminosilane
Tricine	*N*-[tris(hydroxymethyl)methyl]-glycine
Tr	trityl (triphenylmethyl)
Triglyme	triethylene glycol dimethyl ether
Tris	tris(hydroxymethyl)aminomethane
TRITC	tetramethylrhodamine isothiocyanate
TrOC	(see Tcec)
Trp	tryptophan
TRPGDA	tripropylene glycol diacrylate
Ts	tosyl (or *p*-toluenesulfonyl)
Tse	2-*p*-toluenesulfonylethyl
TSIM	*N*-trimethylsilylimidazole
TSNI	1-(*p*-toluenesulfonyl)-4-nitroimidazole
TSP	tribasic sodium phosphate
TSPP	tetrasodium pyrophosphate
TTC	2,3,5-triphenyltetrazolium chloride
TTEGDA	tetraethylene glycol diacrylate
TTF	tetrathiafulvalene
TTFA	thallium(III) trifluoroacetate
TTN	thallium(III) nitrate
Tyr (or Tyr-OH)	tyrosine
Tyr-OMe	tyrosine methyl ester
TX	thromboxane
UDMH	*unsym*-dimethylhydrazine
UDP	uridine 5′-diphosphate
UMP	uridine 5′-monophosphate
UTP	uridine 5′-triphosphate
Val	valine
VMA	4-hydroxy-3-methoxymandelic acid
Voc	vinyloxycarbonyl
VTC	vinyltrichlorosilane
VTEO	vinyltriethoxysilane
VTMO	vinyltrimethoxysilane
VTMOEO	vinyltris(2-methoxyethoxy)silane
XDP	xanthosine 5′-diphosphate
XMP	xanthosine 5′-monophosphate
XTP	xanthosine 5′-triphosphate
Xy	xylene
Z	(see CBn)
Z(Br)	4-bromobenzyloxycarbonyl
Z(NO_2)	4-nitrobenzyloxycarbonyl
Z(OMe)	4-methoxybenzyloxycarbonyl
ZDBC	zinc dibutyldithiocarbamate
ZDEC	zinc diethyldithiocarbamate
ZDMC	zinc dimethyldithiocarbamate
ZPCK	*N*-CBZ-L-phenylalanine chloromethyl ketone

9 Molecular formulae

9.1 The Hill System

In DOC 6, as well as in most other publications including *Chemical Abstracts* and *Beilstein*, molecular formulae are given in Hill system order. For organic compounds, the order is C first, then H, and then the remaining element symbols alphabetically. For compounds that do not contain carbon, the element symbols are ordered alphabetically.

Although the Hill system is now used almost exclusively, other systems have been used in the past. For example, the early formula indexes to *Beilstein* used the Richter system, in which the elements are cited in the order C, H, O, N, Cl, Br, I, F, S, P.

9.2 *Chemical Abstracts* conventions

Users of *Chemical Abstracts* may occasionally have difficulty in locating certain types of compound. For example, sodium acetate will not be found under $C_2H_3NaO_2$; it appears under $C_2H_4O_2$, which is the formula of the parent acid (acetic acid). Conventions that *Chemical Abstracts* uses include the following:

- Metal salts of acids, alcohols and amines are indexed at the molecular formulae of the parent acids, alcohols and amines. Thus, sodium ethoxide appears under C_2H_6O (ethanol) and not under C_2H_5NaO.
- Acid salts of amines (and other basic parents) are indexed at the molecular formulae of the amines. Thus, methanamine hydrochloride appears under CH_5N (methanamine) and not under CH_6ClN.
- Counterions of '-onium' compounds are not included in the formula heading. Thus, 1-methylpyridinium chloride appears under C_6H_8N (1-methylpyridinium) and not under C_6H_8ClN.
- Molecular addition compounds are indexed under the formulae of their components (except that entries are not made for a few common components). Thus, the 1 : 1 addition compound of ethanol with sulfinylbis(methane) (DMSO, dimethyl sulfoxide) appears at C_2H_6O (ethanol) and at C_2H_6OS (sulfinylbismethane) and not at $C_4H_{12}O_2S$.

In general, DOC 6 follows these conventions.

9.3 Checking molecular formulae

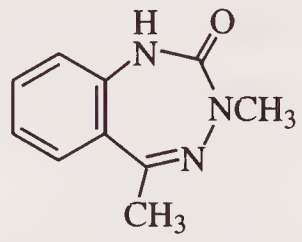
When working out the molecular formula of a neutral organic compound, it is useful to remember that there must be an even number of odd-valent atoms (e.g. H, halogens, N, P). Thus, the formula $C_{27}H_{45}O$ is obviously incorrect unless it is a radical.

A more sophisticated check on the accuracy of a formula is to calculate the number of rings/double bonds in the compound from the formula. You can then count the number of rings and double bonds and compare it with the results of the calculation.

If H = number of univalent atoms (H, halogen), N = number of trivalent atoms (N, P), and C = number of tetravalent atoms, then

$$\text{number of rings/double bonds} = \tfrac{1}{2}(2C - H + N) + 1$$

For example, consider the following:



The formula of this compound is $C_{10}H_{11}N_3O$, i.e. $C = 10$, $H = 11$ and $N = 3$. The formula gives $\frac{1}{2}(20 - 11 + 3) + 1 = 7$, which on inspection of the structure can be seen to be correct (two rings + five double bonds).

The following two points should be noted:

- The number of divalent atoms (O, S) does not

affect the calculation. These must be checked by inspection.

- Triple bonds, including cyano groups, count as two double bonds.

The following version of the equation can be used to work out the number of hydrogen atoms in a molecule (R = number of rings/double bonds):

$$H = 2C + N - 2R + 2$$

or

$$H = 2(C - R + 1) + N$$

10 CAS Registry Numbers

10.1 Introduction

CAS developed the CAS Registry System in the early 1960s to provide a means for determining whether a chemical substance reported in the scientific literature had been indexed previously in *Chemical Abstracts*, and for retrieving the previously assigned index name if it had. Each unique chemical structure recorded in the system is assigned a permanent identifying number, the CAS Registry Number. Originally the Registry System included essentially all substances mentioned in the chemical literature since January 1965 but, in the period 1984–86, CAS assigned Registry Numbers to substances indexed in the Sixth (1957–61) and Seventh (1962–66) Collective Indexes.

10.2 The Registry Number

The CAS Registry Number in itself has no chemical significance, but is simply a serial number assigned as a substance is entered into the Registry System for the first time. The number has the format *NNNNNN–NN–R*, where *R* is a check digit calculated by computer program from the other eight digits; by this means, errors in the transcription of Registry Numbers can be detected. Leading zeros are suppressed, so the first group of digits may contain fewer than six digits.

The check digit for the Registry Number $N_8N_7N_6N_5N_4N_3$–N_2N_1–R is derived from the following formula:

$$\frac{8N_8+7N_7+6N_6+5N_5+4N_4+3N_3+2N_2+N_1}{10} = Q + \frac{R}{10}$$

where Q is an integer, which is discarded.

10.3 Specificity

A substance is registered to the degree of structural detail given. This means that isomers, including stereoisomers, each receive their own Registry Number. Examples are:

25167–67–3	Butene (isomer not specified)
106–98–9	1-Butene
107–01–7	2-Butene (stereoisomer not specified)
624–64–6	(*E*)-2-Butene
590–18–1	(*Z*)-2-Butene
50–21–5	Lactic acid (stereochemistry unspecified)
598–82–3	(±)-Lactic acid (racemic mixture)
10326–41–7	(*R*)-Lactic acid
79–33–7	(*S*)-Lactic acid

Hydrates and salts receive their own Registry Numbers:

302–01–2	Hydrazine
7803–57–8	Hydrazine monohydrate
14011–37–1	Hydrazine hydrochloride
1184–66–3	Hydrazine sulfate

Labelled compounds receive their own Registry Numbers:

64–19–7	Acetic acid (unlabelled)
1112–02–3	Acetic-d_3 acid (D_3CCOOH)
1563–79–2	Acetic-*1*-^{13}C acid ($H_3C^{13}COOH$)

10.4 Duplicate Registry Numbers

CAS sometimes finds it necessary to register substances without a full knowledge of their structures. Examples are trivially named natural products and tradename materials. This may lead to unintentional duplication in the Registry System since the actual material may be indexed at another CA Index Name based on information from another literature source. Similar problems may arise when more than one structure is reported for the same chemical substance. When it is recognised that duplication has occurred and that a substance has been assigned two Registry Numbers, one of the numbers is retained as the preferred number to which the other one is cross-referred.

10.5 Registry Numbers without CA abstract entries

Not all of the substances that have been registered have appeared in CA abstracts or indexes. Thus, it is quite possible to find a Registry Number that does not appear in any CA Substance Index. Some of the sources of these Registry Numbers are:

- In the early years of the Registry System, substances from a number of special data collections such as the Colour Index, Merck Index, Lange Handbook and Pesticide Index were added. Some of these substances may not have been reported subsequently.
- Certain substances are registered for non-CAS use, for example substances registered under the provision of the US Toxic Substances Control Act (TSCA), substances for the USAN (United States Adopted Names) Council of the US Pharmacopeial Convention and substances for the European Inventory of Existing Chemical Substances (EINECS).
- Others arise from the use of the Registry System to support the preparation of index nomenclature. Thus all parent ring systems are registered even when the parent compound has not been made. Also, all components of addition compounds, mixtures or copolymers are registered and, occasionally, one of these components may not have been reported in the literature.

10.6 Registry Numbers with asterisks

CAS, in registering substances for the preparation of CA indexes, assigns Registry Numbers only to substances that are described as unique chemical entities. However, through its activities in the preparation of the TSCA and EINECS inventories, CAS has assigned Registry Numbers to substances that are not treated as unique chemical entities in its regular CA index processing. Registry Numbers assigned to substances of this type are identified by the presence of an asterisk (*) following the number. Examples are:

Tallow (61789–97–7*)
Terphenyl, chlorinated (61788–33–8*)

These Registry Numbers are not found in CA Volume Indexes.

10.7 Registry Numbers and Collective Indexes

Because CA Registry Numbers are assigned sequentially, it is usually possible to tell from the magnitude of a number approximately when it was assigned. Approximate values for the highest CAS Registry Numbers to occur in each CAS Collective Index are as follows:

8CI (1967–71)	35061–04–2
9CI (1972–76)	61690–48–0
10CI (1977–81)	80373–21–3
11CI (1982–86)	106330–30–7
12CI (1987–91)	138463–63–5

Thus a substance with CAS Registry Number 66148–78–5 should appear for the first time in 9CI; certainly, it will not be found in 8CI. However, it should be borne in mind that during 1984–86 CAS registered substances from the Sixth and Seventh Collective Indexes.

For a description of Registry Number policy in DOC 6 see section 2.4.2.

11 Linear notations

A linear notation is a concise means of expressing the structural formula of a chemical compound in a single line of alphabetical and numerical symbols.

The most widely used notation has been the Wiswesser Line-Formula Chemical Notation (WLN, Wiswesser Line Notation). This was once used extensively in systems for the storage and retrieval of information about chemical structures. For example, until 1987 it was used by the Institute for Scientific Information to encode new compounds reported in *Current Abstracts of Chemistry*; these WLNs were then made available through the *Index Chemicus Registry System*. The advent of systems permitting structure or substructure searching using two-dimensional structure diagrams has meant that WLN has declined in importance in recent years, but it can still be used for the generation of connection tables (see below), since many chemists can rapidly encode structures as WLN and algorithms exist to convert WLN to connection tables.

Another notation that is currently used is the Simplified Molecular Input Line Entry System (SMILES). This is the external communication language for the MEDCHEM set of chemical software. It is comparatively easy to encode.

11.1 WLN (Wiswesser Line Notation)

Full details of WLN are given in *The Wiswesser Line-Formula Chemical Notation (WLN)*, 3rd edn, E.G. Smith and P.A. Baker, Chemical Information Management, Cherry Hill, NJ, 1975.

WLN uses 41 symbols: the 10 numerals, 26 capital letters, four punctuation marks (& - / *) and the blank space. All the international atomic symbols are used except K, U, V, W, Y, Cl and Br. Two-letter atomic symbols are enclosed between hyphens, e.g. -SI-. Single letters preceded by a blank space indicate ring positions. Single letters not preceded by a blank space have the following meanings:

C used for a carbon atom only when it is multiply bonded to an atom other than carbon (as in –C≡N or –S–C≡N) or doubly bonded to two other carbon atoms (i.e. the central atom in >C=C=C<)

E bromine atom

F fluorine atom

G chlorine atom

H hydrogen atom – hydrogen atoms are not generally expressed but are understood as part of such symbols as the hydroxyl Q, amino Z and alkyl chain numerals

I iodine atom

J generic halogen; ring closure symbol

K nitrogen atom bonded to more than three other atoms (as in ammonium compounds)

L first symbol of a carbocyclic ring notation

M –NH– group

N nitrogen atom that is hydrogen-free and attached to no more than three other atoms

O oxygen atom that is hydrogen-free (as in ethers)

P phosphorus atom

Q –OH group

R benzene ring

S sulfur atom

T first symbol of a heterocyclic ring notation

U double bond (UU represents a triple bond)

V –C(=O)– (a carbonyl group)

W non-linear dioxygen group as in $-NO_2$ and $-SO_2-$

X carbon atom attached to four atoms other than hydrogen

Y carbon atom attached to three atoms other than hydrogen or doubly bonded oxygen

Z $-NH_2$ group

Numerals preceded by a space show ring sizes if within ring signs; otherwise, numerals show the length of saturated, unbranched alkyl chains.

11.2 SMILES (Simplified Molecular Input Line Entry System)

See D. Weininger, *J. Chem. Inf. Comput. Sci.* 1988, **28**, 31; 1989, **29**, 97 for more information on SMILES.

SMILES is a recently developed line notation that forms part of the MEDCHEM system (marketed by Daylight Chemical Information Systems Inc.). Using simple rules, structures are built as strings of characters. Each atom is shown separately by its atomic symbol; bond symbols are omitted for single bonds; branched structures are shown using nested brackets and rings by assigning numbers to the ring closure bonds, which are specified twice. Aromatic rings are indicated by showing the atom symbols in lower case.

On input SMILES is automatically converted to its canonical form and fragment and substructure searches are also possible.

11.3 Connection tables

A connection table provides a method of describing a chemical structure in a form suitable for processing by computer, permitting structure and substructure searching. A connection table at the basic level represents a structure by listing the atoms and bonds present in a tabular form. Differing levels of sophistication are possible, such as specification of bond type, atom charge, etc. The atom–bond connection table has established itself as the principle form of chemical structure representation for structure databases and computer systems. The commonest form of connection-table format is Molfile from MDL Information Systems, Inc.

12 Hazard information

The hazard information given in DOC 6 has been selected to assist in risk assessments for experimental, manufacturing and manipulative procedures with chemicals.

12.1 Risk and hazard assessment

It is useful to understand the distinction between 'hazard' and 'risk' in the laboratory context. **Hazard** is the set of *inherent properties* of a chemical substance that make it capable of causing adverse effects in people or the environment when a particular degree of exposure occurs. **Risk** is the predicted or actual *frequency of occurrence of an adverse effect* of a chemical substance from a given exposure to humans or the environment. In other words, risk is a function of the physical, reactive and toxic properties of a chemical and the exposure to that substance. Risk assessment therefore requires a knowledge of both the hazard of a chemical and the purpose for which it is being used.

12.2 Physical properties

Physical properties and other quantitative data that are related to the hazard of a chemical and which are quoted in DOC 6, where appropriate, include the following:

- Melting point and boiling point.
- Flash point. Measurements from the closed-cup method are quoted unless only data from the open-cup (oc) method are available. Differing literature flash-point values for the same compound are separated by a slash (/) in DOC 6; the lowest quoted flash point is used for the flammability classification of a chemical.
- Explosive limits. The range in which a mixture of a vapour with air can catch fire or explode on ignition (units: volume per cent (vol%) in air) is given.
- Auto-ignition temperature. This is the lowest temperature at which a substance ignites spontaneously in contact with air and at which the combustion continues without there being a source of ignition (flame or spark). Differing literature auto-ignition temperatures for the same compound are separated by a slash (/) in DOC 6.
- Occupational exposure limits (OELs).

12.3 Occupational exposure limits

In the UK, long-term exposure limits (8 h time-weighted average (TWA) exposures) and short-term exposure limits (STELs, 15 min time-weighted average exposures) are set by the Health and Safety Executive (HSE) and published annually in document EH/40. Two types of exposure limit are defined by the HSE, and these have a different legal status in the UK (e.g. under the Control of Substances Hazardous to Health (COSHH) Regulations 1988).

- A **Maximum Exposure Limit** (MEL) is the maximum concentration of an airborne substance averaged over a reference period to which employees may be exposed by inhalation under any circumstances.
- An **Occupational Exposure Standard** (OES) is the concentration of an airborne substance, averaged over a reference period, at which, according to current knowledge, that is no evidence that it is likely to be injurious to employees if they are exposed by inhalation, day after day, to that concentration.

A substance is assigned an MEL if there are serious implications for the health of those exposed to that material, and a residual risk even at the MEL cannot be discounted. An OES, on the other hand, is set at a level for which there is no indication of a risk to health if exposure occurs daily at that concentration. Recommendations for controlling and monitoring substances assigned MELs and OESs are given in the COSHH Regulations 1988.

Occupational exposure limits are also set by other regulatory and advisory bodies, e.g. Threshold Limit Values (TLVs) by the American Conference of Governmental Industrial Hygienists (ACGIH) and Maximum Arbeitplatz Konzentrations (MAK) by German authorities.

UK occupational exposure limits (ppm or mg m^{-3}) quoted in DOC 6 are taken from the HSE publication EH40/94; the route of exposure is mainly by inhalation, but exposure limits are also assigned to some substances that are easily absorbed by the skin (Sk) or are skin sensitisers (Sen). In the absence of UK data, TLVs published by the ACGIH are provided. Entries for TLVs are either TWA or ceiling (CL) values (CL is a ceiling limit, which must not be exceeded).

12.4 Reactive hazards

For the reactive hazard data, a brief comment is made in DOC 6 on the flammability, explosive (or violent polymerization) properties and the chemical reactivity of a substance, where appropriate.

Flammability classifications are as used in the UK Chemicals (Hazard Information and Packaging) Regulations 1993 (the CHIP regulations) and European Union (EU) legislation, and are based on flash-point (fl.p.) measurements:

- Extremely flammable – liquids with fl.p. < 0 °C and Bp ≤ 35 °C.
- Highly flammable – fl.p. ≥ 0 °C and < 21 °C.
- Flammable – fl.p. ≥ 21 °C and ≤ 55 °C.

No comment is made on substances with fl.p. > 55 °C, but they should be regarded as combustible if brought to a high temperature. Carbon-, sulfur-, nitrogen- and phosphorus-containing chemicals will evolve oxides of their constituent elements, including CO, on combustion, and these gases are toxic and probably irritant if a fire involving such materials is encountered. Similarly, toxic and irritating products will be formed from the decomposition or pyrolysis of some organometallic compounds at elevated temperatures.

Chemical reactivity data include the potential for peroxidation (which may also be indicated by the chemical structure), stability, oxidising/reducing and storage properties, and incompatibility with commonly available chemicals.

12.5 Toxicology

Toxicity information has been chosen to show any likely hazardous effects from short-term or long-term exposure to a substance. Data from human exposure are summarised if available (including possible adverse effects when handling drugs); otherwise experimental (exp.) animal results are quoted, where appropriate.

Local effects on the skin, eyes and respiratory tract plus any systemic toxicity are mentioned in the short-term toxicity data. Acute effects resulting from exposure to high vapour concentrations over a relatively short timescale are also described.

Acute lethality data (LD_{50} by oral or dermal routes of administration, and LC_{50} by inhalation) are quoted for some entries; if oral or skin data have not been reported in the literature, then LD_{50} results from a parenteral route of administration are cited. (Lethal dose 50, LD_{50}, and lethal concentration 50, LC_{50}, are calculated doses and concentrations of a substance expected to cause the death of 50% of an entire defined experimental animal population.) Observations from skin and eye irritation tests are given prominence together with any available human data on irritant or corrosive properties. However, no attempt has been made to distinguish those compounds which are classified as 'mild' irritants experimentally but are not irritating when tested on human volunteers (e.g. cosmetic ingredients).

Chronic toxicity data from long-term or repeated exposure include effects on the skin and respiratory system, target organ toxicity, carcinogenic and reproductive toxic properties.

A chemical is identified in DOC 6 as a *carcinogen* or a *neoplastic agent* either if it appears in Group 1 (human carcinogen), Group 2A (probable human carcinogen) or Group 2B (possible human carcinogen) of the International Agency for Research on Cancer (IARC) classifications or if there is satisfactory evidence that it is an experimental carcinogen or a neoplastic agent. Group 3 compounds from the IARC classification (unclassifiable as to their carcinogenicity to humans) are not listed as such, though their experimental carcinogenic or neoplastic properties are described where appropriate. Experimental carcinogens (and neoplastic agents), which may not yet have been scrutinized by IARC, are classified in some databases (e.g. RTECS) following a critical examination of the experimental

work used to report positive tumorigenic and neoplastigenic findings. Compounds for which there is some doubt about the design of the carcinogenicity test and therefore doubt about their classification are not reported in DOC 6 as 'experimental carcinogens' or 'experimental neoplastic agents'.

Tests on many compounds reveal experimental *reproductive* and/or *teratogenic properties*. The extrapolation and relevance of many of these findings to humans are still problematical. In DOC 6 any experimental effects on the male and female reproductive systems are noted, irrespective of the dose used or the route of administration of the test compound. Similarly, literature reports of teratogenic effects are mentioned, though this term is sometimes used to embrace cases where maternal toxicity has resulted in embryonic or foetal death. A fuller explanation of the observations of reproductive and teratogenic tests quoted in DOC 6 may be found in *Reproductively Active Chemicals: A Reference Guide*, R.J. Lewis, Van Nostrand Reinhold, New York, 1991.

12.6 Health effects of chemicals

Acute data, together with the results of skin and eye irritancy tests and chronic toxicity tests, are required for the hazard classification and labelling of chemicals under EC and UK legislation (e.g. the CHIP regulations and the Notification of New Substances Regulations 1982).

Under the CHIP regulations, the health effects of a chemical are classified from a range of toxicological data:

- Acute lethal effects.
- Non-lethal irreversible effects after a single exposure.
- Severe effects after repeated or prolonged exposure.
- Corrosive effects.
- Irritant effects.
- Sensitising effects.
- Carcinogenic, mutagenic and teratogenic effects.
- Other toxicological properties.

For example, on the basis of either acute lethality data or the type of irreversible but non-lethal damage that may result from a single exposure, chemicals are classified as 'very toxic', 'toxic', or 'harmful'. For classifications from acute lethality studies, the criteria outlined in Table 12.1 apply. Similar dose ranges apply to classifications based on observations of non-lethal irreversible effects following a single exposure.

The CHIP regulations (1993) should be consulted for the criteria that have been adopted to classify other health effects of chemicals, and for risk phrases that are used to describe succinctly these effects.

Different toxicological labels have been applied to acute lethality data in other countries. For example, the phrases 'extremely toxic', 'highly toxic', 'moderately toxic' and 'slightly toxic' are assigned in the USA to the four LD_{50} rat, oral dose ranges 1 mg or less, 1–50 mg, 50–500 mg and 0.5–5 g, respectively. Because of these national variations, LD_{50} data are usually presented in DOC 6 without a toxicity classification. However, exceptions to these guidelines have been made for some particularly hazardous compounds (e.g. those with LD_{50} rat, oral values in the microgram range) and the terms 'very toxic if swallowed', 'very toxic in contact with skin', etc., are used.

Table 12.1 Classification from acute lethality studies

Category[a]	LD_{50} absorbed orally in rat (mg kg^{-1})	LD_{50} absorbed percutaneously in rat or rabbit (mg kg^{-1})	LC_{50} absorbed by inhalation in rat over 4 h (mg l^{-1})
very toxic	≤25	≤50	≤0.5
toxic	>25 to 200	>50 to 400	>0.5 to 2
harmful	>200 to 2000	>400 to 2000	>2 to 20

[a] Qualified by 'if swallowed' for tests by the oral route; 'in contact with skin' for tests by the dermal route; or 'by inhalation'.

12.7 Storage and handling of chemicals

Hazard data – the sum of a substance's physical, reactive and toxic properties – influence the way a chemical should be handled, stored and ultimately discarded.

The safe storage of chemicals requires planning and an appreciation of those chemicals which are incompatible (see Section 12.8). Chemical storage is briefly reviewed in *Chemical Safety Matters*, IUPAC–IPCS, Cambridge University Press, Cambridge, 1992, and a longer account (with a mainly North American regulatory perspective) is given in *Safe Storage of Laboratory Chemicals*, 2nd edn, ed. D.A. Pipitone, Wiley, New York, 1991.

Chemical Safety Matters also provides useful advice on the precautions to be taken when handling those chemicals which present special problems in a laboratory, e.g. substances that have a high acute toxicity or are known to be human carcinogens or can cause other chronic effects.

A more detailed appraisal of the problems of handling carcinogens may be found in *Safe Handling of Chemical Carcinogens, Mutagens, Teratogens and Highly Toxic Substances*, vols 1 and 2, ed. D.B. Walters, Ann Arbor Science, Michigan, 1980, and in the International Agency for Research on Cancer monograph *Handling Chemical Carcinogens in the Laboratory. Problems of Safety*, eds R. Montesano, *et al.*, IARC Scient. Publ. No. 33, IARC, Lyon, 1979.

References to methods for the disposal of chemicals in general, and carcinogens in particular, are provided in Section 12.9.

Awareness of very reactive chemicals is essential. Advice on handling highly flammable and/or potentially explosive reagents is provided in the IUPAC–IPCS book *Chemical Safety Matters*, and the properties of many common but hazardous laboratory chemicals are succinctly summarised in the 'yellow pages' section of *Hazards in the Chemical Laboratory*, 5th edn, ed. S.G. Luxon, Royal Society of Chemistry, Cambridge, 1992. One particular explosive hazard, peroxide-forming chemicals, is described in more detail in Section 12.10.

Handling gases poses special problems for laboratory personnel, from the correct way to store, transport and use compressed gases to the dangers from water being sucked back into the cylinders of hydrolysable gases. *Chemical Safety Matters* provides sound practical advice on using gases, and this book and *Hazards in the Chemical Laboratory* contain summaries of the hazardous and toxic properties of commonly used laboratory gases.

Matheson Gas Products, the USA-based suppliers, have published two useful books on the physical and toxic properties of gases for those who handle them: *Matheson Gas Data Book* 6th edn, W. Braker, *et al.*, 1980 and *Effects of Exposure to Toxic Gases – First Aid and Medical Treatment*, 2nd edn, W. Braker, *et al.*, 1977.

Common to all laboratories are a variety of solvents. Chapter 15 is concerned with the hazardous properties of the most widely encountered solvents.

12.8 Hazardous reaction mixtures

The potential for chemicals to interact in a violent and uncontrolled manner should be foremost in the minds of everyone concerned with the planning and execution of chemical operations. Not only can syntheses and purifications go disastrously wrong if the elementary principles of chemistry are overlooked, but the inadequate storage of incompatible chemicals has led to many a gutted and blackened warehouse and laboratory.

Luckily for the chemist, many of these mishaps of yesteryear have been recorded, most notably by Leslie Bretherick. *Bretherick's Handbook of Reactive Chemical Hazards*, 4th edn, Butterworths, London, 1990, details the predictable and the unexpected from the literature of reactive chemical hazards. In a review, published in *Hazards in the Chemical Laboratory*, 5th edn, ed. S.G. Luxon, Royal Society of Chemistry, Cambridge, 1992, Bretherick has also summarised some frequently encountered incompatible chemicals that present either a reactive hazard or a toxic hazard if combined. These two lists are reprinted here as Tables 12.2 and 12.3 by kind permission of the Royal Society of Chemistry.

12.9 Disposal of chemicals

12.9.1 General guidelines

Guidelines for the safe disposal of small amounts of laboratory chemicals are given in the current edition

Table 12.2 A partial list of incompatible chemicals – *reactive* hazards. Substances in the left-hand column should be stored and handled so that they cannot possibly accidentally contact corresponding substances in the right-hand column under uncontrolled conditions, when violent reactions may occur

acetic acid	chromic acid, nitric acid, peroxides and permanganates
acetic anhydride	hydroxyl-containing compounds, ethylene glycol, perchloric acid
acetone	concentrated nitric and sulfuric acid mixtures, hydrogen peroxide
acetylene	chlorine, bromine, copper, silver, fluorine and mercury
alkali and alkaline-earth metals, such as sodium, potassium, lithium, magnesium, calcium	carbon dioxide, carbon tetrachloride and other chlorinated hydrocarbons (also prohibit water, foam and dry chemical on fires involving these metals – dry sand should be available)
aluminium powder	halogenated or oxygenated solvents
ammonia, anhydrous	mercury, chlorine, calcium hypochlorite, iodine, bromine and hydrogen fluoride
ammonium nitrate	acids, metal powders, flammable liquids, chlorates, nitrites, sulphur, finely divided organics or combustibles
aniline	nitric acid, hydrogen peroxide
bromine	ammonia, acetylene, butadiene, butane and other petroleum gases, sodium carbide, turpentine, benzene and finely divided metals
calcium oxide	water
carbon, activated	calcium hypochlorite, other oxidants
chlorates	ammonium salts, acids, metal powders, phosphorus, sulfur, finely divided organics or combustibles
chromic acid and chromium trioxide	acetic acid, naphthalene, camphor, glycerol, turpentine, alcohol and other flammable liquids
chlorine	ammonia, acetylene, butadiene, butane, other petroleum gases, hydrogen, sodium carbide, turpentine, benzene and finely divided metals
chlorine dioxide	ammonia, methane, phosphine and hydrogen sulfide
copper	acetylene, hydrogen peroxide
fluorine	isolate from everything
hydrazine	hydrogen peroxide, nitric acid, any other oxidant, heavy-metal salts
hydrocarbons (benzene, butane, propane, gasoline, turpentine, etc.)	fluorine, chlorine, bromine, chromic acid, conc. nitric acid, peroxides
hydrogen cyanide	nitric acid, alkalis
hydrogen fluoride	ammonia, aqueous or anhydrous
hydrogen peroxide	copper, chromium, iron, most metals or their salts, any flammable liquid, combustible materials, aniline, nitromethane
hydrogen sulfide	fuming nitric acid, oxidising gases
iodine	acetylene, ammonia (anhydrous or aqueous)
mercury	acetylene, fulminic acid[a], ammonia
nitric acid (conc.)	acetic acid, acetone, alcohol, aniline, chromic acid, hydrogen cyanide, hydrogen sulfide, flammable liquids, flammable gases, nitratable substances, fats, grease
nitromethane, lower nitroalkanes	inorganic bases, amines, halogens, 13X molecular sieve
oxalic acid	silver, mercury, urea
oxygen	oils, grease, hydrogen, flammable liquids, solids or gases
perchloric acid	acetic anhydride, bismuth and its alloys, alcohol, paper, wood, grease, oils, dehydrating agents
peroxides, organic	acids (organic or mineral), avoid friction, store cold
phosphinates	any oxidant
phosphorous (white)	air, oxygen
potassium chlorate	acids (see also chlorates)
potassium perchlorate	acids (see also perchloric acid)
potassium permanganate	glycerol, ethylene glycol, benzaldehyde, sulfuric acid
silver	acetylene, oxalic acid, tartaric acid, fulminic acid[a], ammonium compounds
sodium	see alkali metals (above)
sodium nitrite	ammonium nitrate and other ammonium salts

Table 12.2 *Continued*

sodium peroxide	any oxidisable substrate, such as ethanol, methanol, glacial acetic acid, acetic anhydride, benzaldehyde, carbon disulfide, glycerol, ethylene glycol, ethyl acetate, methyl acetate and furfural
sulfuric acid	chlorates, perchlorates, permanganates
thiocyanates	metal nitrates, nitrites, oxidants
trifluoromethanesulfonic acid	perchlorate salts

[a] Produced in nitric acid–ethanol mixtures.
Reproduced with permission from L. Bretherick, *Hazards in the Chemical Laboratory*, (ed. S.G. Luxon); published by the Royal Society of Chemistry, 1992.

of the *Aldrich Catalogue Handbook of Fine Chemicals*, and a more detailed account of waste disposal management may be found in *Handbook of Laboratory Waste Disposal*, M.J. Pitt, *et al.*, Ellis Horwood, Chichester, 1985.

Detailed experimental procedures have been published on how to convert particularly reactive and toxic substances into less harmful products before their disposal; see for example *Hazardous Laboratory Chemicals Disposal Guide*, M.A. Armour, CRC Press, Boca Raton, FL, 1991.

Destruction of Hazardous Chemicals in the Laboratory, 2nd edn, G. Lunn, *et al.*, Wiley, Chichester, 1994, contains methods for the degradation and disposal of the following chemicals:

acid halides and anhydrides
aflatoxins
alkali and alkaline-earth metals
alkali-metal alkoxides
antineoplastic alkylating agents
aromatic amines
azides
azo and azoxy compounds and tetrazenes
biological stains
boron trifluoride and inorganic fluorides
butyllithium
calcium carbide
carbamic acid esters
chloromethylsilanes and silicon tetrachloride
N-chlorosuccinimide
chlorosulfonic acid
Cr(VI)
cisplatin
citrinin

Table 12.3 A partial list of incompatible chemicals – *toxic* hazards. Substances in the left-hand column should be stored and handled so that they cannot possibly accidentally contact corresponding substances in the centre column, because toxic materials (right-hand column) would be produced

arsenical materials	any reducing agent[a]	arsine
azides	acids	hydrogen azide
cyanides	acids	hydrogen cyanide
hypochlorites	acids	chlorine or hypochlorous acid
nitrates	sulfuric acid	nitrogen dioxide
nitric acid	copper, brass, any heavy metals	nitrogen dioxide (nitrous fumes)
nitrites	acids	nitrous fumes
phosphorus	caustic alkalis or reducing agents	phosphine
selenides	reducing agents	hydrogen selenide
sulfides	acids	hydrogen sulfide
tellurides	reducing agents	hydrogen telluride

[a] Arsine has been produced by putting an arsenical alloy into a wet galvanized bucket.
Reproduced with permission from L. Bretherick, *Hazards in the Chemical Laboratory*, (ed. S.G. Luxon); published by the Royal Society of Chemistry, 1992.

complex metal hydrides
cyanides and cyanogen bromide
cycloserine
dichloromethotrexate, vincristine and vinblastin
diisopropyl fluorophosphate
dimethyl sulfate and related compounds
doxorubicin and daunorubicin
drugs containing hydrazine and triazene groups
ethidium bromide
haloethers
halogenated compounds
halogens
heavy metals
hexamethylphosphoramide
hydrazines
hypochlorites
mercury
methotrexate
2-methylaziridine
1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP)
mitomycin C
4-nitrophenyl
N-nitrosamines and *N*-nitrosamides
nitrosourea drugs
ochratoxin A
organic nitriles
OsO_4
patulin
peracids
peroxides and hydroperoxides
phosgene
phosphorus and P_4O_{10}
picric acid
polycyclic aromatic and heterocyclic hydrocarbons
$KMnO_4$
β-propiolactone
protease inhibitors
$NaNH_2$
sterigmatocystin
sulfonyl fluoride enzyme inhibitors
6-thioguanine and 6-mercaptopurine
uranyl compounds

Methods for the conversion of the major classes of chemical carcinogens into non-mutagenic residues are also described in a series of monographs published by the International Agency for Research on Cancer. A summary of this work is available, and an adapted version is reproduced in Section 12.9.2 by kind permission of the Royal Society of Chemistry.

Disposal methods for some of the more common classes of organic compounds may be found in *Chemical Safety Matters* (hydrocarbons, halogenated hydrocarbons, alcohols and phenols, ethers, thiols and organosulfur compounds, carboxylic acids and derivatives, aldehydes, ketones, amines, nitro and nitroso compounds and peroxides).

12.9.2 Experimental details for the degradation of carcinogens

The material presented in this section has been adapted from Castegnaro, M., *The Laboratory Environment*, ed. R. Purchase, Royal Society of Chemistry, Cambridge, 1994, pp. 91–112. This is a condensed version and Castegnaro gives alternative methods for some classes of compounds.

(*a*) Aflatoxins and other mycotoxins

Validated methods

(i) For aflatoxins. 20 ml of sodium hypochlorite solution (5% available chlorine) are sufficient to degrade 20 µg of pure aflatoxins. Other components in the waste may also react with sodium hypochlorite. It is recommended, therefore, that the efficiency of the degradation of the aflatoxins is checked. An adequate excess of sodium hypochlorite should be used. A similar procedure using NaOCl can be used for sterigmatocystin, citrinin and ochratoxin.

(ii) 10 ml of 0.3 mol l^{-1} potassium permanganate in 2 mol l^{-1} sodium hydroxide will degrade 400 µg of patulin, 300 µg of sterigmatocystin or aflatoxins B1, B2, G1 or G2 and 2 mg of citrinin or ochratoxin, in 3 h. Other components in the waste may react with potassium permanganate, turning the purple/green colour to brown.

References

Castegnaro, M., Friesen, M., Michelon, J. and Walker, E.A., *Am. Ind. Hyg. Assoc. J.*, 1981, **42**, 398.

Laboratory Decontamination and Destruction of Aflatoxins B_1, B_2, G_1, G_2 in Laboratory Wastes, eds M. Castegnaro, D.C. Hunt, E.B. Sansone, P.L. Schuller, M.G. Siriwardana, G.M. Telling, H.P. Van Egmond and E.A. Walker. IARC Scient. Publ. No. 37, IARC, Lyon, 1980.

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some Mycotoxins, eds M. Castegnaro, J. Barek, J.M. Fremy,

M. Lafontaine, M. Miraglia, E.B. Sansone and G.M. Telling. IARC Scient. Publ. No. 113, IARC, Lyon, 1991.

(*b*) *N*-Nitrosamines

Validated methods

(i) A solution of the *N*-nitrosamine in dichloromethane or another suitable solvent is concentrated, dried and treated with an excess of hydrobromic acid solution (3%) on the basis that 5 ml of the HBr solution is sufficient to degrade 1 mg of *N*-nitrosamine in 1–2 ml of solvent within 15 min. Of the nitrosamines tested, *N*-nitrosopyrrolidine is an exception, requiring 10 ml of hydrobromic acid solution to degrade 1 mg in 90 min. The rate of reaction is drastically decreased by the presence of water or dimethyl sulfoxide (DMSO).

(ii) 50 ml of potassium permanganate (0.3 mol l^{-1}) in sulfuric acid (3 mol l^{-1}) will degrade a mixture containing approx. 300 µg of *N*-nitrosamines. Other components in the waste may react with potassium permanganate (turning the purple colour to brown). Thus in all cases sufficient permanganate should be added to maintain a permanent purple colour.

(iii) 50 g of nickel–aluminium alloy (50/50) are sufficient to destroy 5 g of *N*-nitrosamines in 1 litre of 0.5 mol l^{-1} potassium hydroxide. Other components in the waste may also react with the nickel–aluminium alloy or may poison the nickel catalyst that is formed. It is recommended, therefore, that the efficiency of the degradation is checked.

References

Castegnaro, M., Michelon, J. and Walker, E.A., in N-*Nitroso Compounds: Occurrence and Biological Effects*, eds H. Bartsch, I.K. O'Neill, M. Castegnaro and M. Okada. IARC Scient. Publ. No. 41, IARC, Lyon, 1982, p. 151.

Chien, R.T. and Thomas, M.H., *J. Environ. Pathol. Toxicol.*, 1978, **2**, 513.

Emmet, G.C., Michejda, C.I., Sansone, E.B. and Keefer, L.K., in *Safe Handling of Chemical Carinogens, Mutagens, Teratogens and Highly Toxic Substances*, ed. D.B. Walters. Ann Arbor Science, Michigan, 1979, p. 535.

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some N-*Nitrosamines*, eds M. Castegnaro, G. Eisenbrand, G. Ellen, L. Keefer, D. Klein, E.B. Sansone, D. Spincer, G.M. Telling and K. Webb. IARC Scient. Publ. No. 43, IARC, Lyon, 1982.

Lunn, G., Sansone, E.B. and Keefer, L.K., *Food Chem. Toxicol.*, 1981, **19**, 493.

Lunn, G., Sansone, E.B. and Keefer, L.K., *Carcinogenesis*, 1983, **4**, 315.

(*c*) Polycyclic aromatic and heterocyclic compounds (PAC and PHC)

Validated methods

(i) 10 ml of a solution containing 0.3 mol l^{-1} potassium permanganate in 3 mol l^{-1} sulfuric acid will degrade 5 mg of PAC or PHC in acetone in 1 h. Other components in the wastes may react with potassium permanganate, turning the purple colour to brown. It is recommended, therefore, that the efficiency of the degradation is checked.

(ii) For PAH and some PHC. 10 ml concentrated sulfuric acid will degrade 5 mg of PAH dissolved in 2 ml DMSO in 2 h. The efficiency of destruction depends upon the ratio of sulfuric acid:DMSO, and this should not be less than 5:1. In other solvents such as acetone and DMF, the reaction was found to proceed satisfactorily for most PAH/PHC, but longer reaction periods were required.

(iii) For PHC. 5 mg PHC in 5 ml of acetone are completely degraded by treatment for about 1 h with 0.2 to 0.3 g iron(II) chloride and 10 ml H_2O_2.

References

Castegnaro, M., Coombs, M., Phillipson, M.A., Bourgade, M.C. and Michelon, J., in *Proceedings of the 7th Symposium on Polynuclear Hydrocarbons*, Springer-Verlag, New York, 1983, p. 257.

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some Polycyclic Aromatic Hydrocarbons, eds M. Castegnaro, G. Grimmer, O. Hutzinger, W. Karcher, H. Kunte, M. Lafontaine, E.B. Sansone, G. Telling and S.P. Tucker. IARC Scient. Publ. No. 49, IARC, Lyon, 1983.

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some Polycyclic Heterocyclic Compounds, eds M. Castegnaro, J. Barek, J. Jacob, U. Kirso, M. Lafontaine, E.B. Sansone, G.M. Telling and T. Vu Duc, IARC Scient. Publ. No. 114, IARC, Lyon, 1991.

Lunn, G., Sansone, E.B., De Méo, M., Laget, M. and Castegnaro, M., *Am. Ind. Hyg. Assoc. J.*, 1994, **55**, 167.

(*d*) Nitrosamides

Compounds investigated include: *N*-nitroso-*N*-methylurea and *N*-nitroso-*N*′-nitro-*N*-methylguanidine.

Validated methods

(i) 35 g of iron filings in 1 litre of solution containing 3 mol l^{-1} hydrochloric acid are sufficient to destroy 17 g *N*-nitrosamides. Other components in the waste may interfere with the destruction process, so it is recommended that the efficiency of the degradation is checked. This method must not be used in the presence of acetone.

(ii) 10 ml of a solution containing 0.3 mol l^{-1} potassium permanganate in 3 mol l^{-1} sulfuric acid will degrade 50 mg of nitrosamide within 8 h. Although the actual chemical degradation takes much less time, it is necessary to allow the reaction to proceed for 8 h to obtain non-mutagenic residues. This method must not be used for shorter periods.

(iii) A solution of 100 mg *N*-nitrosamides in 2 ml dry dichloromethane, ethyl acetate or any other suitable solvent is concentrated and treated with 10 ml of a solution of 3% hydrobromic acid to give quantitative degradation of *N*-nitrosamides within 15 min. The NOBr formed is removed by flushing with nitrogen for 30 min. The rate of reaction is drastically reduced by the presence of water or alcohols.

References

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some N-Nitrosamides, eds M. Castegnaro, M. Bernard, L.W. Van Broekhoven, D. Fine, R. Massey, E.B. Sansone, P.L.R. Smith, B. Spiegelhalder, A. Stacchini and J.J. Vallon. IARC Scient. Publ. No. 55, IARC, Lyon, 1984.

Lunn, G. and Sansone, E.B., *Food Chem. Toxicol.*, 1988, **26**, 481.

Lunn, G., Sansone, E.B., Andrews, A.W., Castegnaro, M., Malaveille, C., Michelon, J., Brouet, I. and Keefer, L.K., in N-*Nitroso Compounds: Occurrence, Biological Effects and Relevance to Human Cancer*, eds I.K. O'Neill, R.C. Von Borstel, C.T. Miller, J. Long and H. Bartsch. IARC Scient. Publ. No. 57, IARC, Lyon, 1984.

(*e*) Hydrazines

Validated methods

(i) 50 g of nickel–aluminium alloy (50/50) are sufficient to destroy 5 g of hydrazines in 1 litre of 0.5 mol l^{-1} potassium hydroxide. Other compounds in the waste may also react with the nickel–aluminium alloy or may poison the nickel catalyst that is formed. It is recommended, therefore, that the efficiency of the degradation is checked. Addition of nickel–aluminium alloy to an alkaline solution results in a highly exothermic reaction with the evolution of large quantities of hydrogen. It is essential to add the alloy slowly over a period of time while cooling the reaction vessel in an ice bath. Care should be taken that the nickel–aluminium alloy powder is kept in suspension throughout the operation (avoid lumps or adherence to sides of the reaction vessel).

(ii) Other methods described for destruction of hydrazines use acid potassium permanganate, acid potassium iodate or calcium hypochlorite.

References

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some Hydrazines, eds M. Castegnaro, G. Ellen, M. Lafontaine, H.C. Van der Plas, E.B. Sansone and S.P. Tucker. IARC Scient. Publ. No. 54, IARC, Lyon, 1983.

Lunn, G., Sansone, E.B. and Keefer, L.K., *Environ. Sci. Technol.*, 1983, **17**, 240.

(*f*) Haloethers

Validated methods

(i) In water-miscible solvents, 1 ml of 6% ammonia will degrade 50 mg of chloromethyl methyl ether or bis(chloromethyl) ether in 3 h. In water-immiscible solvents, 1 ml of 33% ammonia will degrade 50 mg of haloether in 3 h.

(ii) 3.5 ml of 15% m/v sodium phenate in methanol will degrade 50 mg of chloroether in 1 ml of solvent in 3 h.

(iii) 1.5 ml of a 8–9% m/v sodium methoxide in methanol will degrade 50 mg of chloroether in 1 ml of solvent in 3 h.

References

Alvarez, M. and Rosen, R.T., *Int. J. Environ. Anal. Chem.*, 1976, **4**, 241.

Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some Haloethers, eds M. Castegnaro, M. Alvarez, M. Iovu, E.B. Sansone, G.M. Telling and D.T. Williams. IARC Scient. Publ. No. 61, IARC, Lyon, 1984.

(*g*) Aromatic amines and 4-nitrobiphenyl

Validated methods

(i) Amine dissolved in 10 ml of 0.1–1.0 mol l^{-1} hydrochloric acid at a concentration of 0.005 mol l^{-1}, or in glacial acetic acid at a concentration of 0.001 mol l^{-1}, is degraded by the action of 5 ml

potassium permanganate (0.2 mol l^{-1}) and 5 ml sulfuric acid (2 mol l^{-1}) within 10 h.

(ii) Other methods described use H_2O_2/peroxidase, Zn/H_2SO_4 or diazotisation with $NaNO_2$ followed by basification.

References

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Lunn, G. and Sansone, E.B., *Appl. Occup. Environ. Hyg.*, 1991, **6**, 49.

(*h*) Antineoplastic agents and other drugs

Compounds investigated include the following: doxorubicin, daunorubicin, methotrexate, dichloromethotrexate, cyclophosphamide, ifosfamide, vincristine sulfate, vinblastine sulfate, 6-thioguanine, 6-mercaptopurine, streptozotocin, chlorozotocin, lomustine, carmustine, PCNU, semustine, melphalan, dacarbazine, uracil mustard, procarbazine, spiromustine, isoniazid, iproniazid and mechlorethamine.

Validated methods

(i) For doxorubicin and daunorubicin. 30 mg of doxorubicin or daunorubicin dissolved in 10 ml of 3 mol l^{-1} sulfuric acid are degraded by 1 g potassium permanganate during 2 h. Very slight mutagenic activity has been detected from this degradation of doxorubicin.

(ii) For methotrexate and dichloromethotrexate. 50 mg of methotrexate or 10 mg of dichloromethotrexate (solid) dissolved in 10 ml of 3 mol l^{-1} sulfuric acid are degraded by 0.5 g potassium permanganate in 1 h. In the case of pharmaceutical preparations containing dichloromethotrexate, up to 50 mg can be dissolved in 10 ml of 3 mol l^{-1} sulfuric acid and degraded with 0.5 g potassium permanganate.

(iii) For methotrexate. 50 mg of methotrexate, dissolved in 50 ml of 4% m/v sodium hydroxide, are degraded by 5.5 ml of 1% m/v potassium permanganate in 30 min.

(iv) For methotrexate. 50 mg of methotrexate dissolved in 100 ml of 4% m/v sodium hydroxide are degraded by 4.6 ml of 5.25% sodium hypochlorite in 30 min.

(v) For cyclophosphamide and ifosfamide. 10 ml of 12% m/v sodium hydroxide are sufficient to degrade 100 mg cyclophosphamide or ifosfamide in 20 ml DMF, when refluxed for 4 h.

(vi) For cyclophosphamide. A sample of 250 mg cyclophosphamide dissolved in 10 ml of 1 mol l^{-1} hydrochloric acid is completely hydrolysed when refluxed for 1 h. After addition of 1.5 g sodium thiosulfate to the neutralized reaction mixture, the medium is made strongly alkaline with 20% m/v sodium hydroxide and the reaction allowed to proceed for 1 h.

(vii) For vincristine sulfate and vinblastine sulfate. 10 mg of vincristine sulfate or vinblastine sulfate in 10 ml of 3 mol l^{-1} sulfuric acid are completely degraded by 0.5 g potassium permanganate in 2 h.

(viii) For 6-thioguanine and 6-mercaptopurine. 18 mg of 6-thioguanine or 6-mercaptopurine dissolved in 20 ml of 3 mol l^{-1} sulfuric acid are degraded by 0.13 g potassium permanganate in 10–12 h.

(ix) For lomustine, chlorozotocin and streptozotocin. 100 mg of lomustine dissolved in 2–3 ml dichloromethane, or 100 mg solid chlorozotocin or streptozotocin, are degraded by 10 ml of a 4.5% solution of hydrobromic acid in glacial acetic acid in 15 min. The nitrosyl bromide formed is removed by flushing with nitrogen for 30 min to prevent possible re-formation of *N*-nitrosoureas.

(x) For streptozotocin. 48 mg of streptozotocin dissolved in 10 ml of 3 mol l^{-1} sulfuric acid are degraded by 2 g potassium permanganate in 10–12 h.

(xi) Other, non-validated methods are described in the references cited.

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Laboratory Decontamination and Destruction of Carcinogens in Laboratory Wastes: Some Hydrazines, eds M. Castegnaro, G. Ellen, M. Lafontaine, H.C. Van Der Plas, E.B. Sansone and S.P. Tucker. IARC Scient. Publ. No. 54, IARC, Lyon, 1983.

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Monteith, D.K., Connor, T.H., Benvenuto, J.A., Fairchild, E.J. and Theiss, J.C., *Environ. Mol. Mutagen.*, 1987, **10**, 341.

Monteith, D.K., Connor, T.H., Benvenuto, J.A., Fairchild, E.J. and Theiss, J.C., *Toxicol. Lett.*, 1988, **40**, 257.

(*i*) Some alkylating agents

Compounds investigated include: dimethyl sulfate (DMS), diethyl sulfate (DES), methyl methanesulfonate (MMS) and ethyl methanesulfonate (EMS).

Methods not validated

(i) For DMS. 13.3 g of DMS in 500 ml of 1 mol l^{-1} sodium hydroxide, or 1 mol l^{-1} sodium carbonate, or 1.5 mol l^{-1} ammonium hydroxide, are hydrolysed in 15 min. 0.1 ml of DMS in 1 ml methanol, ethanol, dimethylsulfoxide (DMSO), acetone, or dimethylformanide (DMF) are hydrolysed by treatment with 4 ml of one of the above-mentioned alkaline solutions for 15 min (for methanol, ethanol, DMSO, or DMF solution) or 1 h (for acetone solutions). 0.1 ml of DMS in 1 ml toluene, *p*-xylene, benzene, 1-pentanol, ethyl acetate chloroform or carbon tetrachloride are degraded by shaking with 4 ml of one of the above-mentiond alkaline solutions for 1 day.

(ii) For DMS, DES, MMS and EMS. The compounds are degraded with 1 mol l^{-1} $Na_2S_2O_3$ according to the kinetic formula $\ln C = \ln C_0 - at$, where C_0 is the initial concentration of alkylating agent, a is a constant dependent on the compound to be degraded and the reaction temperature, and t is time (in minutes). At 25 °C, $a = 4.85$ (DMS), 0.73 (DES), 1.16 (MMS), 0.12 (EMS). Thus 99.5% degradation is achieved in 1 min for DMS, 7 min (DES), 1.6 min (MMS) and 44 min (EMS).

References

De Méo, M., Laget, M., Castegnaro, M. and Duménil, G., *Am. Ind. Hyg. Assoc. J.*, 1990, **51**, 505.

Lunn, G. and Sansone, E.B., *Am. Ind. Hyg. Assoc. J.*, 1985, **46**, 111.

(*j*) Azo and azoxy compounds and 2-aminoanthracene

Compounds investigated include: azobenzene, azoxyanisole, phenylazophenol, phenylazoaniline, Fast Garnet and 2-aminoanthracene.

Methods not validated

(i) For azobenzene, azoxyanisole, phenylazophenol, phenylazoaniline, 2-aminoanthracene and Fast Garnet. To 10 mg of compound (5 mg for phenylazoaniline) in 1 ml glacial acetic acid, add 40 ml (80 ml for phenylazoaniline) of 0.3 mol l^{-1} potassium permanganate in 3 mol l^{-1} sulfuric acid. Stir at room temperature for 18 h.

Table 12.4 Types of chemicals that may form peroxides

Organic structures
ethers and acetals with α-hydrogen atoms
olefins with allylic hydrogen atoms
chloroolefins and fluoroolefins
vinyl halides, esters and ethers
dienes
vinylacetylenes with α-hydrogen atoms
alkylacetylenes with α-hydrogen atoms
alkylarenes that contain tertiary hydrogen atoms
alkanes and cycloalkanes that contain tertiary hydrogen atoms
acrylates and methacrylates
secondary alcohols
ketones that contain α-hydrogen atoms
aldehydes
ureas, amides and lactams that have a H atom linked to a C attached to a N
Inorganic substances
alkali metals, especially potassium, rubidium and a caesium
metal amides
organometallic compounds with a metal atom bonded to carbon
metal alkoxides

(ii) For azobenzene, azoxybenzene, azoxyanisole and phenylazophenol. To a 5 mg ml–1 solution in methanol, add an equal volume of 2 mol l–1 potassium hydroxide and 1 g of nickel–aluminium alloy (50/50) per 20 ml of mixture. Allow to react while stirring at room temperature for 18 h.

(iii) For all compounds. Stir 10 ml of a saturated aqueous solution with 0.5 g Amberlite XAD-16 for 18 h and then filter.

Reference

Lunn, G. and Sansone, E.B., *Appl. Occup. Environ. Hyg.*, 1991, **6**, 1020.

Table 12.5 Common peroxide-forming chemicals

Severe peroxide hazard on storage with exposure to air. *Discard within 3 months*

- diisopropyl ether
- divinylacetylene[a]
- potassium metal
- sodium amide (sodamide)
- vinylidene chloride (1,1-dichloroethylene)[a]
- potassium amide

Peroxide hazard on concentration: do not distil or evaporate without first testing for the presence of peroxides. *Discard or test for peroxides after 6 months*

- acetaldehyde diethyl acetal (1,1-diethoxyethane)
- cumene (isopropylbenzene)
- cyclohexene
- cyclopentene
- decalin (decahydronaphthalene)
- diacetylene (1,3-butadiyne)
- dicyclopentadiene
- diethyl ether (ether)
- diethylene glycol dimethyl ether (diglyme)
- dioxan/dioxolan (dioxane)
- ethylene glycol dimethyl ether (glyme)
- ethylene glycol ether acetates
- ethylene glycol monoethers (cellosolves)
- furan
- methylacetylene
- methylcyclopentane
- methyl isobutyl ketone
- tetrahydrofuran
- tetralin (tetrahydronaphthalene)
- vinyl ethers[a]

Hazard of rapid polymerization initiated by internally formed peroxides[a]

(A) Normal liquids. *Discard or test for peroxides after 6 months*[b]

- chloroprene (2-chloro-1,3-butadiene)[c]
- styrene
- vinyl acetate
- vinylpyridine

(B) Normal gases. *Discard after 12 months*[d]

- butadiene[c]
- tetrafluoroethylene[c]
- vinylacetylene[c]
- vinyl chloride

[a] Monomers may polymerize and should be stored with a polymerization inhibitor from which the monomer can be separated by distillation just before use.

[b] Although common acrylic monomers such as acrylonitrile, acrylic acid, ethyl acrylate and methyl methacrylate can form peroxides, they have not been reported to develop hazardous levels in normal use and storage.

[c] The hazard from peroxide formation in these compounds is substantially greater when they are stored in the liquid phase.

[d] Although air cannot enter a gas cylinder in which gases are stored under pressure, these gases are sometimes transferred from the original cylinder to another in the laboratory, and it is difficult to be sure that there is no residual air in the receiving cylinder. An inhibitor should be put into any secondary cylinder before transfer. The supplier can suggest an appropriate inhibitor to be used. The hazard posed by these gases is much greater if there is a liquid phase in the secondary container. Even inhibited gases that have been put into a secondary container under conditions that create a liquid phase should be discarded within 12 months.

12.10 Peroxide-forming chemicals

Peroxide-forming solvents and reagents should be dated at the time they are first opened, and should be either discarded or tested for peroxides within a fixed period of time after their first use.

Peroxides can be detected with NaI/AcOH, though dialkyl peroxides may need treatment with conc. HCl or 50% H_2SO_4 before detection with iodide is possible. A commercially available test paper, which contains a peroxidase, can detect hydroperoxides and dialkyl peroxides, as well as oxidizing anions, in organic and aqueous solvents.

Hydroperoxides, but not dialkyl peroxides, can be removed from peroxide-forming solvents by passage through basic activated alumina, by treatment with a self-indicating activated molcular sieve (type 4A) under nitrogen, or by treatment with Fe^{2+}/H^+, CuCl, or other reductants.

Methods for the detection and removal of peroxides from organic solvents are summarised in *Organic Solvents: Physical Properties and Methods of Purification*, 4th edn, eds J.A. Riddick *et al.*, Wiley, Chichester, 1986. The deperoxidation of ethers with molecular sieve is described by Burfield, D.R., *J. Org. Chem.*, 1982, **47**, 3821. An exhaustive review of the determination of organic peroxides is available: Mair, R.D., *et al.*, in *Treatise on Analytical Chemistry*, eds I.M. Kolthoff *et al.*, Interscience, New York, 1971, vol. 14, part II, p. 295.

The types of structures that have been identified as likely to produce peroxides are listed in Table 12.4, and some common peroxidisable chemicals are quoted in Table 12.5. Tables 12.4 and 12.5 are reproduced with permission from IUPAC–IPCS, *Chemical Safety Matters*, Cambridge University Press, Cambridge, 1992 and the American Chemical Society.

12.11 Conclusion

One of the aims of DOC 6 is to provide basic hazard data; exhaustive coverage of, for example, the *in vivo*, *in vitro* and environmental toxicology of a substance is not possible. Neither does the omission of hazard information in DOC 6 imply its absence from the literature. Widely recognised hazards are included, however, and, where possible, critically assessed toxicity reviews (tox rev) of chemicals are identified in the references supplied for each entry. These reviews should be consulted for the extrapolation of animal toxicity data to people when making risk assessments, and for other hazard data.

To end on a cautionary note. Lack of hazard information does not mean that the consequences of handling a chemical can be disregarded. Any chemical has the capacity for harm if it is carelessly used, and, for many newly synthesised materials (e.g. new synthetic reagents), hazardous properties may not be apparent or may not have been cited in the literature. (For example, methyl fluorosulfonate (Magic Methyl) was in extensive use before it was found to be very highly toxic.) In addition, the toxicity of some very reactive chemicals may not have been evaluated because of ethical considerations.

Good laboratory and manufacturing practices (now increasingly encoded in national and international legislation) place emphasis on the key attitudes to be adopted when working with chemical substances (or mixtures):

- Prevention of exposure (by elimination or substitution).
- Control of exposure.
- Monitoring exposure.
- Maintenance of control measures.
- Health surveillance.
- The provision of hazard information.

12.12 Further reading

Risk and hazard assessment (general)

Compiler's Guide for the Preparation of International Chemical Safety Cards, Commission of the European Communities, Luxembourg, 1990.

King, R., *Safety in the Process Industries*, Butterworth-Heinemann, London, 1990.

Steere, N.V., in *Laboratory Safety: Theory and Practice*, eds A.A. Fuscaldo, B.J. Erlick and B. Hindman. Academic Press, New York, 1980, pp. 3–28 (the concept of injury resulting from a transfer of energy).

Toxic Hazard Assessment of Chemicals, ed. M.L. Richardson. Royal Society of Chemistry, London, 1986 (definitions of risk and hazard).

Physical properties

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Kirk-Othmer's Encyclopedia of Chemical Technology, 3rd & 4th edns, Wiley, New York, 1983 & 1991.

Riddick, J.A. *et al.*, *Organic Solvents: Physical Properties and Methods of Purification*, 4th edn, Wiley-Interscience, New York, 1986 (vapour pressure relationships, flash points, etc.).

Stephenson, R.M., *Flash Points of Organic and Organometallic Compounds*, Elsevier, Amsterdam, 1987.

Verschueren, K., *Handbook of Environmental Data on Organic Chemicals*, 2nd edn, Van Nostrand Reinhold, New York, 1983.

Occupational exposure limits

EH40/94 Occupational Exposure Limits 1994, HMSO, London, 1993.

Occupational Exposure Limits for Airborne Toxic Substances, 3rd edn, ILO, Geneva, 1991 (data from 16 countries).

Threshold Limit Values and Biological Exposure Indices for 1992–1993, American Conference of Governmental Industrial Hygienists, Ohio, 1992.

Reactive hazards

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn, Butterworth, Sevenoaks, 1990.

Hazards in the Chemical Laboratory, 5th edn, ed. S.G. Luxon. Royal Society of Chemistry, London, 1992.

Jackson, H.L., *et al.*, *J. Chem. Educ.*, 1970, **47**, A175 (peroxidisable compounds).

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BIBRA Toxicity Profiles, BIBRA, Carshalton, 1986–.

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Ethel Browning's Toxicity and Metabolism of Industrial Solvents, vols 1–3, 2nd edn, ed. R. Snyder, Elsevier, Amsterdam, 1987–1992.

Grandjean, P., *Skin Penetration: Hazardous Chemicals at Work*, Taylor & Francis, London, 1990 (300 chemicals that are poisonous by skin absorption).

Hathaway, G.J., *et al.*, *Proctor and Hughes' Chemical Hazards of the Workplace*, 3rd edn, Van Nostrand Reinhold, New York, 1991.

IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans, Supplement 7, IARC, Lyon, 1987.

Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold, New York, 1989.

Lewis, R.J., *Reproductively Active Chemicals: A Reference Guide*, Van Nostrand Reinhold, New York, 1991.

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn, Van Nostrand Reinhold, New York, 1992 ('Sax'; LD_{50} and LC_{50} data, carcinogenic and reproductive toxicity properties).

Martindale, the Extra Pharmacopoeia, 30th edn, Pharmaceutical Press, London, 1993 (adverse effects of therapeutic agents).

Proctor, N.H., *et al.*, *Chemical Hazards of the Workplace*, 2nd edn, Van Nostrand Reinhold, New York, 1988.

Registry of Toxic Effects on Chemical Substances (RTECS), The National Institute for Occupational Safety and Health (NIOSH), Ohio. (RTECS is available on a quarterly updated CD-ROM (Chem-Bank), which also includes other health and safety databanks, from SilverPlatter International NV.)

Teratogens, 2nd edn, ed. V.M. Kolb, Elsevier, Amsterdam, 1993.

Health and safety data sheets

Chemical Safety Sheets, Kluwer Academic, Dordrecht, 1991 (includes a section on the prediction of chemical handling properties from physical data).

Compendium of Safety Data Sheets for Research and Industrial Chemicals, ed. L.H. Keith, VCH, Deerfield Park, 1987.

Dictionary of Substances and their Effects (DOSE), eds M.L. Richardson, *et al.*, Royal Society of Chemistry, Cambridge, 1992.

Hazard Data Sheets, BDH, Poole, Dorset.

Hazardous Chemicals Data Book, 2nd edn, ed. G. Weiss. Noyes Data, USA, 1986.

Hazards in the Chemical Laboratory, 5th edn, ed. S.G. Luxon. Royal Society of Chemistry, London, 1992.

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Improving Safety in the Chemical Laboratory: A Practical Guide, 2nd edn, ed. J.A. Young, Wiley, New York, 1991.

IUPAC–IPCS, *Chemical Safety Matters*, Cambridge University Press, Cambridge, 1992 (useful laboratory safety advice including storage and disposal of waste chemicals).

Health and safety legislation

Safe Practices in Chemical Laboratories, Royal Society of Chemistry, London, 1989 (Section F of this booklet summarises the main provisions of the Health and Safety at Work Act 1974, subsequent Regulations made under the Act (including the Control of Substances Hazardous to Health Regulations 1988), and other legislation affecting laboratories).

Selwyn, N., *Law of Health and Safety at Work*, Butterworths, London, 1982.

Tolley's Health and Safety at Work Handbook 1992–1993, ed. M. Dewis. Tolley, Croydon, 1992.

13 Languages

The best dictionaries for chemists are:

Patterson, A.M., *German–English Dictionary for Chemists*, Wiley, Chichester.
Patterson, A.M., *French–English Dictionary for Chemists*, Wiley, Chichester.
Dictionary of Chemical Terminology in Five Languages, Elsevier, Amsterdam, 1980 (covers English, German, French, Polish and Russian).

13.1 A German–English dictionary

Note that the correct form of many German words ending in 'ss' is to use the symbol 'ß', e.g. 'Blaß', 'Heiß'. Since this symbol is frequently not available on keyboards and complicates indexing, it is becoming less frequent, but will still often be found in books and journals.

For use on keyboards without an umlaut, or where it is desired to avoid use of the umlaut, the correct transiteration is to insert a following e, e.g. Tröger's base → Troeger's base.

Abbau	decomposition, degradation
abdestillieren	to distil off
aber	but, however
abfiltrieren	to filter off
abgeben	to give off
abkühlen	to cool down
abnehmend	decreasing
Abscheidung	separation
abtrennen	to separate
Abtrennung	separation
Abweichung	deviation, variation
acht	eight
ähnlich	similar
Alkylierung	alkylation
allgemein	generally
allmählich	gradual(ly)
als	as, then
alt	old
Ameisensäure	formic acid
ander	other, another
ändern	to change
anders	otherwise, differently
anfänglich	at first
anfangs	at first
angesäuert	acidified
Angriff	attack
Anlagerung	addition, approach
annähernd	approximate
ansäuern	to acidify
anstelle	instead
Anteil	constituent
Anwendung	use
Anwesenheit	presence
Äpfelsäure	malic acid
Äthanol	ethanol
Äther	ether
äthyl	ethyl
auch	also
Aufarbeitung	work up
auffangen	to collect
auflösen	to dissolve
Aufnahme	absorption
aus	out of, from
Ausbeute	yield
ausfällen	to precipitate
ausführen	to carry out
Ausgangsmaterial	starting material
ausgenommen	except
ausgeschieden	separated
Ausscheidung	separation
Ausschluss	exclusion
ausser	except, besides
ausserdem	besides, moreover
Bad	bath
basisch	basic
Bedeutung	meaning, significance
behandeln	to treat
Beispiel	example
bekannt	known
Belichtung	exposure to light
Benzin	petroleum ether
Benzol	benzene
beobachten	to observe
berechnet	calculated

bereiten	to prepare
bereits	already
Bernsteinsäure	succinic acid
beschleunigen	to accelerate
beschreiben	to describe
besonders	especially
besser	better
beständig	stable
Bestandteil	constituent
bestehen	to consist, to exist
bestimmen	to determine
Bestimmung	determination
Bestrahlung	irradiation
Beugung	diffraction
beweisen	to prove
bilden	to form
Bildung	formation
Bindung	bond
bis	until
blass	pale
Blatt	leaf
Blättchen	leaflet
blau	blue
bläulich	bluish
Blausäure	hydrocyanic acid
Blei	lead
Bor	boron
brauchbar	useful
braun	brown
bräunlich	brownish
Brechung	refraction
Breite	width
brennen	to burn
Brenztraubensäure	pyruvic acid
Brom	bromine
Bromierung	bromination
Brücke	bridge
Buttersäure	butyric acid
Chinolin	quinoline
Chinon	quinone
Chlor	chlorine
Chlorierung	chlorination
Chlorwasserstoff	hydrogen chloride
dagegen	on the other hand
Dampf	vapour
danach	after that
daneben	besides
darin	therein, in it
Darstellung	preparation
dass	that
Dehydratisierung	dehydration
Dehydrierung	dehydrogenation
Derivat	derivative
desgleichen	likewise
destillieren	to distil
Destillierung	distillation
deutlich	clear
dick	thick
dies	this
diese	this, these
digerieren	to digest
doppelt	double
drei	three
dreifach	triple
dreissig	thirty
Druck	pressure
dunkel	dark
dünn	thin
durch	through, by
durchführen	to carry out
ebenfalls	likewise
Eigenschaft	property
ein	one
einbringen	to introduce
eindampfen	to evaporate
eindeutig	unequivocal
einengen	to concentrate
einfach	simple
einiger	some, several
Einkristall	single crystal
einleiten	to introduce
einmal	once
Einschluss	inclusion
einstündig	for one hour
eintägig	for one day
eintropfen	to add dropwise
einzig	only
Eis	ice
Eisen	iron
Eisessig	glacial acetic acid
elf	eleven
eluieren	to elute
Enolisierung	enolisation
entfernen	to remove
entgegen	against
enthalten	to contain
entsprechend	corresponding
entstehen	to originate
Entwässerung	dehydration

Entwicklung	evolution
Entzündung	ignition
erfolgen	to occur
erforderlich	necessary
ergeben	to yield
Ergebnis	result
ergibt	yields
erhalten	to obtain
erhitzen	to heat
Erhöhung	increase
erscheinen	to appear
erst	first, only
Erstarrung	solidification
erste	first
erwärmen	to warm
erzielen	to obtain
Essigsäure	acetic acid
fällen	to precipitate
falsch	incorrect
Farbe	colour
farbig	coloured
farblos	colourless
Farbstoff	dyestuff
Farbumschlag	colour change
fast	almost
fein	fine
Feld	field
ferner	further
fest	solid
Feststoff	solid
Feuchtigkeit	moisture
Flammpunkt	flash point
flüchtig	volatile
flüssig	liquid
Flüssigkeit	liquid
Folge	sequence, series
folgen	to follow
Formel	formula
Fortschritt	progress
frei	free
frisch	fresh
früher	former(ly)
führen	to lead
fünf	five
ganz	whole
Gärung	fermentation
gasförmig	gaseous
geben	to give
gebräuchlich	usual
gebunden	bonded
geeignet	suitable
gefällt	precipitated
gefärbt	coloured
Gefäss	vessel
gegen	against
Gegenwart	presence
Gehalt	contents
gekocht	boiled
gekühlt	cooled
gelb	yellow
gelblich	yellowish
gelöst	dissolved
Gemisch	mixture
gemischt	mixed
genau	exact
gepuffert	buffered
gering	small
geringer	minor
Geruch	odour
gerührt	stirred
gesättigt	saturated
geschmolzen	fused, molten
Geschwindigkeit	rate
getrennt	separated
getrocknet	dried
Gewicht	weight
gewinnen	to obtain
gewiss	certainly
gewogen	weighed
gewöhnlich	usual
gibt	gives
giftig	poisonous, toxic
Gitter	lattice
gleich	equal
gleichfalls	likewise
Gleichgewicht	equilibrium
Gleichung	equation
gleichzeitig	simultaneously
gliedrig	membered
grau	grey
Grenze	limit
gross	great, large
grün	green
Gruppe	group
halb	half
Halogenierung	halogenation
haltbar	stable
Harnstoff	urea
Hauptprodukt	main product

heftig	violently
heiss	hot
hell	light, pale
hemmen	to inhibit
Herkunft	origin
herstellen	to produce
Herstellung	production
Hilfe	help
hingegen	on the contrary
hinzufügen	to add
Hitze	heat
hoch	high
hohe	high
hundert	hundred
Hydratisierung	hydration
Hydrierung	hydrogenation
immer	always
induziert	induced
Inhalt	contents
insgesamt	altogether
Isolierung	isolation
Jahr	year
je nach	according to
jedoch	however
Jod	iodine
Jodierung	iodination
Kalium	potassium
kalt	cold
katalytisch	catalytic
kein	no, not a
Kern	nucleus
Kette	chain
klar	clear
klein	small
kochen	to boil
Kochpunkt (Kp)	boiling point (Bp)
Kohlensäure	carbon dioxide, carbonic acid
Kohlenstoff	carbon
Kohlenwasserstoff	hydrocarbon
kondensieren	to condense
konjugiert	conjugated
konzentriert (konz.)	concentrated (conc.)
Kopplung	coupling
Kraft	force
Kühlen	to cool
kühlung	cooling
Kupfer	copper
kurz	short
Ladung	charge
lang	long
langsam	slow(ly)
lassen	to leave
leicht	easy, easily
leiten	to conduct
letzte	last
Licht	light
liefern	to yield
links	left
lösen	to dissolve
löslich	soluble
Löslichkeit	solubility
Lösung	solution
Lösungsmittel	solvent
Luft	air
mässig	moderately
mehr	more
mehrere	several
mehrfach	multiple
mehrmals	several times
mehrstündig	for several hours
meist	most
Menge	amount
Messung	measurement
Milchsäure	lactic acid
mischbar	miscible
Mischbarkeit	miscibility
mischen	to mix
Mischung	mixture
mit	with
mittels	by means of
möglich	possible
Molverhältnis	molar ratio
müssen	must
Mutterlauge	mother liquor
nach	after
nachfolgend	subsequent
nachstehend	following
Nacht	night
Nachweis	proof, detection
Nadel	needle
nahe	near
nämlich	namely
Natrium	sodium
neben	beside, in addition to
Nebenprodukt	by-product
neun	nine
Niederschlag	precipitate

niedrig	low
niemals	never
Nitrierung	nitration
noch	still, yet
nochmalig	repeated
notwendig	necessary
nunmehr	now
nur	only
oben	above
Oberfläche	surface
oberhalb	above
oder	or
offen	open
offenbar	obvious
ohne	without
Öl	oil
ölig	oily
Ölsäure	oleic acid
Phosphor	phosphorus
primär	primary
protoniert	protonated
Puffer	buffer
Pulver	powder
Punkt	point
Quecksilber	mercury
rasch	rapid
Raum	space, room
rechts	right
Reihe	series
rein	pure
Reinheit	purity
Reinigung	purification
restlich	residual
richtig	correct
Rohprodukt	crude product
rosa	pink
rot	red
rötlich	reddish
Rückfluss	reflux
Rückgewinnung	recovery
Rückstand	residue
rühren	to stir
Salpetersäure	nitric acid
Salz	salt
Salzsäure	hydrochloric acid
sättigen	to saturate
sauer	acidic
Sauerstoff	oxygen
Säure	acid
Schall	sound
scheiden	to separate
scheinbar	apparently
schlecht	poor
schliessen	to close
schliesslich	finally
schmelzen	to melt
Schmelzpunkt (Schmp)	melting point (Mp)
schnell	fast, quickly
schon	already
schütteln	to shake
Schutzgas	inert gas
schwach	weak
schwarz	black
Schwefel	sulfur
Schwefelsäure	sulfuric acid
schwer	heavy, difficult
Schwingung	vibration
sechs	six
sehr	very
Seitenkette	side-chain
sieben	seven
sieden	to boil
siedend	boiling
Siedepunkt	boiling point
Silizium	silicon
sofort	immediately
sonst	otherwise, else
sorgfältig	carefully
Spaltung	cleavage, scission
Spiegel	mirror
Stäbchen	small rod
stark	strong
starr	rigid
statt	instead of
stattfinden	to take place
stehen	to stand
stehen lassen	to leave standing
Stellung	position
Stickstoff	nitrogen
Stoff	substance
Stoffwechsel	metabolism
Stoss	impact, collision
Strahlung	radiation
streuen	to scatter
Stufe	step, stage
Stunde	hour

substituiert	substituted
Tafel	plate
Täfelchen	platelet
Tag	day
Teil	part
Teilchen	particle
teilweise	partially
tief	deep
Toluol	toluene
trennen	to separate
Trennung	separation
trocken	dry
trocknen	to dry
Tropfen	drop
über	over, above
Übergang	transition
Überschuss	excess
überwiegend	predominantly
üblich	usual
übrig	remaining
Umesterung	transesterification
Umkristallisierung	recrystallisation
Umlagerung	rearrangement
Umsatz	exchange
Umsetzung	reaction
Umwandlung	conversion
unbeständig	unstable
unkorrigiert	uncorrected
unlöslich	insoluble
unrein	impure
unten	below, underneath
unter	under
Untersuchung	investigation
ursprünglich	original
Verbindung	compound
Verbrennung	combustion
Verdampfung	evaporation, vaporisation
verdünnt (verd.)	dilute (dil.)
vereinigen	to combine
Veresterung	esterification
Verfahren	procedure
verfärben	to change colour
Vergärung	fermentation
Vergleich	comparison
vergleichen	to compare
Verhalten	behaviour
Verhältnis	proportion, ratio
Verlauf	course, progress
vermindern	to diminish, to reduce
vermischen	to mix
verrühren	to stir up
Verschiebung	shift
Verseifung	saponification
versetzen	to add, mix
Versuch	experiment
verwandt	related
Verwendung	use
verzweigt	branched
viel	much, many
vielleicht	perhaps, possibly
vier	four
voll	full
vom	of the, from the
vor allem	above all
Vorbehandlung	pretreatment
Vorkommen	occurrence
Vorsicht	caution, care
vorsichtig	cautious(ly)
vorwiegend	predominant
wahrscheinlich	probable, probably
waschen	to wash
Wasser	water
Wasserdampf	water vapour, steam
wasserfrei	anhydrous
wasserhaltig	hydrated or wet
wässerig	aqueous
Wasserstoff	hydrogen
wässrig	aqueous
Weg	route
wegen	on account of
Weinsäure	tartaric acid
weiss	white
weiter	additional
Welle	wave
Wellenlänge	wavelength
wenig	little, few
werden	to become
Wertigkeit	valency
wesentlich	essential
wichtig	important
wiederholt	repeated(ly)
Winkel	angle
wird	becomes, is
Wirkung	action, effect
Wismut	bismuth
Woche	week
zehn	ten

Zeit	time
Zeitschrift	periodical, journal
zerfliesslich	deliquescent
zersetzen	to decompose
zersetzlich	unstable
Zersetzung (Zers.)	decomposition (dec.)
ziegelrot	brick red
Zimmer	room
Zimtsäure	cinnamic acid
Zinn	tin
Zucker	sugar
zuerst	at first
zufügen	to add
Zugabe	addition
zugebeu	to add
zugleich	at the same time, together
zuletzt	at last, finally
zum Beispiel (z.B.)	for example (e.g.)
Zunahme	increase
zur	to the
zurückbleiben	to remain behind
zusammen	together
zusäzlich	additional
Zustand	state, condition
zutropfen	to add drop by drop
zuvor	before, previously
zwanzig	twenty
zwecks	for the purpose of
zwei	two
zweimal	twice
zwischen	between
Zwischenprodukt	intermediate
zwölf	twelve

13.2 Russian–English transliteration

A system for transliterating Russian is shown in Table 13.1.

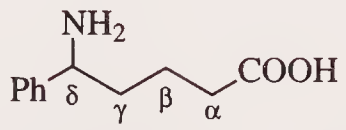
Table 13.1 A Russian–English transliteration table

Russian capital	Russian small	English equivalent
А	а	a
Б	б	b
В	в	v
Г	г	g
Д	д	d
Е	е	e
Ё	ё	e
Ж	ж	zh
З	з	z
И	и	i
Й	й	i
К	к	k
Л	л	l
М	м	m
Н	н	n
О	о	o
П	п	p
Р	р	r
С	с	s
Т	т	t
У	у	u
Ф	ф	f
Х	х	kh
Ц	ц	ts
Ч	ч	ch
Ш	ш	sh
Щ	щ	shch
Ъ	ъ	’
Ы	ы	y
Ь	ь	’
Э	э	e
Ю	ю	yu
Я	я	ya

13.3 The Greek alphabet in organic chemistry

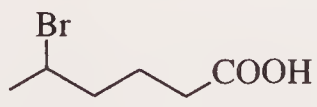
All Greek letters are used in alphabetical order for the following purposes:

- Numbering of chains, especially in conjunctive nomenclature. (Note that the COOH carbon is *not* included.)



δ-aminobenzenepentanoic acid

- For compounds not subject to conjunctive nomenclature, the α,β,... numbering is found in the older literature but is now obsolete.



δ-bromocaproic acid (obsol.)
≡ 5-bromohexanoic acid

Table 13.2 Applications of the Greek alphabet in organic chemistry documentation

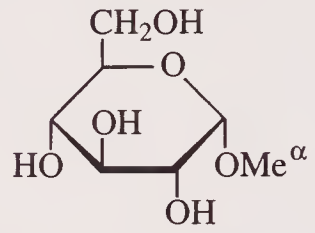
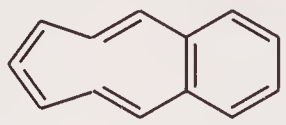
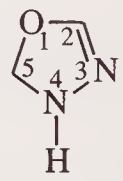
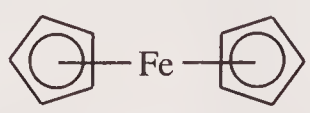
Capital	Lower-case	Name	Applications
A	α	alpha	Optical rotation. α without brackets refers to an experimentally measured rotation value, e.g. α = –19.2° (obsol.). α in square brackets refers to the specific rotation of a compound in a given solvent and at the experimental temperature, e.g. $[\alpha]_D^{25}$ –57.4 (c. 0.25 in $CHCl_3$); it is a dimensionless number and a degree sign should *not* be used. Concentrations are given in g/100 ml Indicates below-the-plane stereochemistry in steroids, terpenoids, etc., e.g. 5α-pregnane Indicates configuration of the glycosidic bond in glycosides  methyl α-D-glucopyranoside
B	β	beta	Indicates above-the-plane stereochemistry in steroids, terpenoids, etc., e.g. 5β-pregnane Indicates configuration of the glycosidic bond in glycosides, e.g. methyl β-D-glucopyranoside A descriptor for carotenoid end-groups
Γ	γ	gamma	
Δ	δ	delta	Lower-case delta (δ) is used to indicate the presence of a contiguous double bond in a cyclic parent. Thus $8\delta^2$-benzocyclononene indicates that two double bonds terminate at atom 8 in the benzocyclononene ring system (*Pure Appl. Chem.*, 1988, **60**, 1395)  $8\delta^2$-benzocyclononene Upper-case delta (Δ) with a superscript locant denotes the presence and position of a double bond  Δ^2-1,3,4-oxadiazoline
E	∈ or ε	epsilon	Absorption maximum or minimum amplitude in uv/visible spectroscopy, e.g. λ_{max} 550 nm (∈ 10 500) (often expressed logarithmically) A descriptor for carotenoid end-groups
Z	ζ	zeta	
H	η	eta	Indicates coordination number in organometallic chemistry  bis(η^5-cyclopentadienyl)iron (ferrocene) Viscosity

Table 13.2 *Continued*

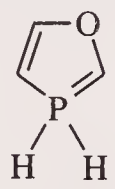
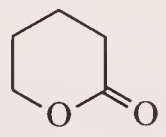
Capital	Lower-case	Name	Applications
Θ	θ	theta	In cd (circular dichroism) spectroscopy
I	ι	iota	
K	κ	kappa	A descriptor for carotenoid end-group
Λ	λ	lambda	Absorption or trough wavelength in uv/visible and cd spectroscopy (see under ∈ and θ above) Denotes unusual (higher) valency in a chemical structure, especially in compounds of third-row elements  1,3λ^5-oxaphosphole
M	μ	mu	Abbreviation for *meso*- as in μ-tartaric acid (obsol.)
N	ν	nu	Frequency in infrared spectroscopy
Ξ	ξ	xi	Lower-case xi (ξ) denotes unknown configuration at a chiral centre (alternative to α,β or *R*,*S*), e.g. 1β,2β,3ξ-trihydroxy-12-ursen-23-oic acid. In Beilstein, Ξ is used in place of D or L where the configuration is uncertain
O	o	omicron	
Π	π	pi	Delocalised bond type derived essentially for p orbital overlap
P	ρ	rho	
Σ	σ	sigma	Bond type derived nominally from s orbital overlap
T	τ	tau	In pmr spectroscopy; old fashioned, $\tau = 10 - \delta$
Y	υ	upsilon	
Φ	ϕ or φ	phi	Abbreviation (obsol.) for phenyl, C_6H_5 Carotenoid end-group descriptor
X	χ	chi	Carotenoid end-group descriptor
Ψ	ψ	psi	Abbreviation for 'pseudo-', e.g. pseudoakuammigine or ψ-akuammigine Carotenoid end-group descriptor
Ω	ω	omega	The last carbon atom of a chain. Positions proximate to the end of the chain can be indicated as, for example, Δ(ω – 4) alkenoic acids

Table 13.3 Greek and Latin multiplicative prefixes

	Greek	Latin
1/2	hemi	semi
1	mono, mon	uni
3/2		sesqui
2	di	bi
3	tri	tri, ter
4	tetra, tetr	quadri, quadr, quater
5	penta, pent	quinque, quinqu
6	hexa, hex	sexi, sex
7	hepta, hept	septi, sept
8	octa, oct, octo, octi	
9	ennea, enne	nona, non, novi
10	deca, dec, deci	
11	hendeca, hendec	undeca, undec
12	dodeca, dodec	
13	trideca, tridec	
14	tetradeca, tetradec	
15	pentadeca, pentadec	
16	hexadeca, hexadec	
17	heptadeca, heptadec	
18	octadeca, octadec	
19	nonadeca, nonadec	
20	eicosa, eicos (or ic...)	
21	henicosa, henicos	
22	docosa, docos	
23	tricosa, tricos	
24	tetracosa, tetracos	
25	pentacosa, pentacos	
26	hexacosa, hexacos	
27	heptacosa, heptacos	
28	octacosa, octacos	
29	nonacosa, nonacos	
30	triconta, triacont	
31	hentriconta, hentriacont	
32	dotriaconta, dotriacont	
33	tritriaconta, tritriacont	
40	tetraconta, tetracont	
50	pentaconta, pentacont	
60	hexaconta, hexacont	
70	heptaconta, heptacont	
80	octaconta, octacont	
90	nonaconta, nonacont	
100	hecta, hect	
101	henhecta, henhect	
102	dohecta, dohect	
110	decahecta, decahect	
120	eicosahecta, eicosahect (or ic...)	
132	dotriacontahecta, dotriacontahect	
200	dicta, dict	
300	tricta	
400	tetracta	
1000	kilia	

- To indicate lactone ring size (obsol.), as derived from the position of the –OH group in the parent hydroxyacid above.



δ-valerolactone

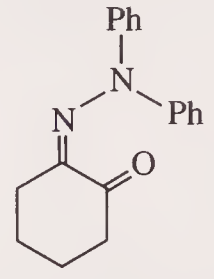
- Greek letters have an important colloquial use to refer to positions in a molecule or class of molecules, e.g. 'α- to the carbonyl group', 'β,γ-unsaturated ketones', etc.
- Where stereochemistry of a series of isomers is unknown, Greek labels α, β,... are often used arbitrarily to distinguish them (e.g. the isomers α to θ of 1,2,3,4,5,6-hexachlorocyclohexane, configurations now largely known).
- To denote polymorphic forms, especially in crystallography.

Other specific uses of Greek letters in organic chemistry are listed in Table 13.2.

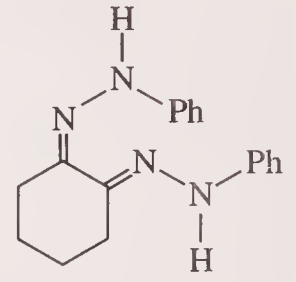
13.4 Multiplicative prefixes from Greek and Latin

In CAS index names, Greek prefixes are preferred, except for sesqui- (for one and one-half), nona- (for nine) and undeca- (for eleven). The terms hemi- (Greek) and sesqui- (Latin) are employed by CAS only in hydrate and ammoniate names. A full list is given in Table 13.3.

The terms bis, tris, tetrakis, etc. (meaning essentially 'twice', 'three times', etc.) are used to avoid ambiguity in nomenclature. This is best illustrated by the following example.



1,2-cyclohexanedione diphenylhydrazone (strictly, mono(diphenylhydrazone))



1,2-cyclohexanedione bis(phenylhydrazone)

14 SI units

14.1 Basic SI units

The names and symbols for the SI base units are shown in Table 14.1.

Table 14.1 SI base units

Physical quantity	Unit name	Unit symbol
amount of substance	mole	mol
electric current	ampere	A
length	metre	m
luminous intensity	candela	cd
mass	kilogram	kg
temperature	kelvin	K
time	second	s

14.2 Common derived SI units

The approved special names and symbols for some derived SI units are shown in Table 14.2.

14.3 Prefixes used with SI units

The prefixes listed in Table 14.3 may be used to indicate decimal multiples of base and derived SI units.

Table 14.2 SI derived units

Physical quantity	Unit name	Unit symbol	Definition
charge	coulomb	C	A s
energy	joule	J	$kg\ m^2\ s^{-2}$
force	newton	N	$kg\ m\ s^{-2} = J\ m^{-1}$
frequency	hertz	Hz	s^{-1}
potential difference	volt	V	$kg\ m^2\ s^{-3}\ A^{-1} = J\ A^{-1}\ s^{-1}$
power	watt	W	$kg\ m^2\ s^{-3} = J\ s^{-1}$
pressure	pascal	Pa	$kg\ m^{-1}\ s^{-2} = N\ m^{-2}$

Table 14.3 Multiplying prefixes for use with SI units

Factor	Prefix	Symbol	Factor	Prefix	Symbol
10^{-1}	deci	d	10	deca	da
10^{-2}	centi	c	10^2	hecto	h
10^{-3}	milli	m	10^3	kilo	k
10^{-6}	micro	μ	10^6	mega	M
10^{-9}	nano	n	10^9	giga	G
10^{-12}	pico	p	10^{12}	tera	T
10^{-15}	femto	f	10^{15}	peta	P
10^{-18}	atto	a	10^{18}	exa	E
10^{-21}	zepto[a]	z	10^{21}	zetta[a]	Z
10^{-24}	yocto[a]	y	10^{24}	yotta[a]	Y

[a] Proposed in *Chem. Int.*, 1992, **14**, 100.

14.4 Conversion factors

Length

1 ångstrom unit (Å) = 10^{-8} cm = 10^{-10} m
= 10^{-1} nm
1 micron (μ) = 1 μm = 10^{-4} cm = 10^{-6} m
A wavelength of n microns (n μm) ≡ a wavenumber of 10 000/n cm^{-1}
2.54 cm = 1 inch (in)
1 metre = 39.3701 inches

Mass

453.592 g = 1 pound (lb)
1 kg = 2.20462 lb

Volume

1 ml (or 1 mL) = 1 cubic centimetre (cm^3)
1 litre = 2.12 pints (US) = 1.76 pints (UK)
28.6 ml = 1 fluid ounce

Pressure

1 atm = 1.01325×10^5 pascal (N m^{-2})
= 101.325 kPa
= 760 torr = 760 mmHg
= 1.01325 bar
= 14.70 lb/in^2
1 mmHg (0 °C) = 1 torr = 1/760 atm
= 133.322 pascal
= 0.0193368 lb/in^2
1 kPa = 7.5006 mmHg
1 lb/in^2 = 51.715 mmHg

Temperature

absolute zero (K) = −273.16 °C
K = °C + 273.16
°F = (9 × °C)/5 + 32
°C = 5 (°F − 32)/9

Energy

1 joule = 1 watt s = 10^7 erg = 0.737561 ft lb
1 erg = 1 dyne cm = 1 g cm^2 s^{-2}
1 calorie = 4.1868 joule
1 electronvolt/molecule = 23.06 kcal mol^{-1}

15 Commonly used solvents

15.1 Boiling points and fire hazards

Solvents are given in Table 15.1 in order of increasing boiling point to the nearest 1 °C. The hazard information given refers to *flammability* only. **Many solvents pose a toxic hazard**. Severe potential toxic hazards are marked ▷(OES long-term exposure limit <100 ppm). Readers should consult the more detailed hazard/toxicity information given in DOC 6 and references cited there before using a solvent for the first time. For further information on some of the more common solvents, see *Organic Solvents: Physical Properties and Methods of Purification*, 4th edn, J.A. Riddick, *et al.*, Wiley, Chichester, 1986.

15.2 Handling solvents

A variety of solvents are handled and stored in all physical- and life-science laboratories. Although their presence may be familiar and, like other laboratory chemicals, they are subject to control by health and safety regulations, caution is necessary, when using solvents. Apart from the acute effects of high concentrations of the more volatile solvents, the possible neurotoxic and carcinogenic implications of long-term exposure to low levels of various solvents are also of concern. The physical properties of some of the common laboratory solvents are referred to in Section 15.1.

Recent publications on the hazards of solvents are listed below:

Bond, J., *Sources of Ignition*, Butterworth, Oxford, 1991.

Chemical Safety Data Sheets, vol. 1, *Solvents*, Royal Society of Chemistry, Cambridge, 1989.

Durrans, T.H., *Solvents*, 8th edn, ed. E.H. Davies, Chapman & Hall, London, 1971.

Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn, ed. R. Snyder, Elsevier, Amsterdam, vols 1, 2, 3, 1987, 1990, 1992.

Greim, H., *et al.*, *Chemical Carcinogens*, 2nd edn, ed. C.E. Searle, ACS Monograph 182, vol. 1, p. 525, American Chemical Society, Washington, DC, 1984 (carcinogenicity).

Henning, H. (ed.), *Solvent Safety Sheets: A Compendium for the Working Chemist*, Royal Society of Chemistry, Cambridge, 1993.

Long-Term Neurotoxic Effects of Paint Solvents. Royal Society of Chemistry, London, 1993 (neurotoxicity).

Luxon, S.G. (ed.) *Hazards in the Chemical Laboratory*, 5th edn, Royal Society of Chemistry, Cambridge, 1992, chapter 4 (health and safety regulations).

Table 15.1 Fire hazard of some common solvents

Bp (°C)	Mp (°C)	DOC Name[a]	Flash point (°C)	Hazard[b]
30–60		petrol[c]		extremely flammable
30	–161	2-methylbutane	<–51	extremely flammable
32	–99	methyl formate	<–19	extremely flammable
35	–116	diethyl ether	–45	extremely flammable
36	–129	pentane	–49	extremely flammable
38	–98	dimethyl sulfide	–34	highly flammable
40	–97	dichloromethane		conc. 12–19% in air, flammable
46	–112	▶carbon disulfide	–30	extremely flammable
46	–14	1,1,1-trichloro-2,2,2-trifluoroethane		non-flammable
47	–111	1,2-dibromo-1,1,2,2-tetrafluorethane		non-flammable
50	–94	cyclopentane	–37	extremely flammable

Table 15.1 *Continued*

Bp (°C)	Mp (°C)	DOC Name[a]	Flash point (°C)	Hazard[b]
54	–109	2-methoxy-2-methylpropane	–28	highly flammable
56	–94	acetone	–17	highly flammable
56	–98	methyl acetate	–9	highly flammable
61	–63	▶chloroform		non-flammable
65	–108	▶tetrahydrofuran	–14	highly flammable
65	–98	methanol	10	highly flammable
69	–87	diisopropyl ether	–28	highly flammable
69	–94	hexane	–23	highly flammable
72	–15	▶trifluoroacetic acid		non-flammable
74	–32	▶1,1,1-trichloroethane		non-flammable
75	–95	1,3-dioxolane	2	highly flammable
77	–84	ethyl acetate	–4	highly flammable
77	–21	▶carbon tetrachloride		non-flammable
78	–117	ethanol	12	highly flammable
78	–123	1-chlorobutane	–12	highly flammable
80	–86	2-butanone	1	highly flammable
80	6	▶benzene	–11	highly flammable
81	6	cyclohexane	–20	highly flammable
82	–45	▶acetonitrile	6	highly flammable
82	–90	2-propanol	12	highly flammable
83	26	2-methyl-2-propanol	10	highly flammable
84	–35	1,2-dichloroethane	13	highly flammable
85	–58	1,2-dimethoxyethane	–6	highly flammable
87	–85	▶trichloroethylene		non-flammable
88	–45	tetrahydropyran	–20	highly flammable
97	–127	1-propanol	15	highly flammable
98	–92	heptane	–4	highly flammable
99	–108	2,2,4-trimethylpentane	–12	highly flammable
100	–115	2-butanol	24	highly flammable
100	0	water		non-flammable
101	11	▶1,4-dioxane	11	highly flammable
101	–127	methylcyclohexane	–4	highly flammable
101	–29	▶nitromethane	35	flammable
101	8	formic acid	69	
102	–42	3-pentanone	13	highly flammable
103	15	trimethyl orthoformate	15	highly flammable
104	–6	bromotrichloromethane		non-flammable
108	–108	2-methyl-1-propanol	28	flammable
111	–95	toluene	4	highly flammable
114	–36	▶1,1,2-trichloroethane		non-flammable
116	–42	▶pyridine	20	flammable
117	–80	4-methyl-2-pentanone	17	highly flammable
118	–90	1-butanol	29	flammable
118	17	▶acetic acid	39	flammable
121	–19	▶tetrachloroethylene		non-flammable
125	–86	▶2-methoxyethanol	43	flammable
126	–77	▶butyl acetate	22	flammable
126	–57	octane	13	highly flammable
132	–117	3-methyl-1-butanol	43	flammable
132	10	▶1,2-dibromoethane		non-flammable
132	–45	▶chlorobenzene	24	flammable

Table 15.1 *Continued*

Bp (°C)	Mp (°C)	DOC Name[a]	Flash point (°C)	Hazard[b]
135	–70	2-ethoxyethanol	44	flammable
136	–94	ethylbenzene	15	highly flammable
138	14	1,4-dimethylbenzene	25	flammable
139	–47	1,3-dimethylbenzene	25	flammable
142	–79	isopentyl acetate	23	flammable
142	–98	dibutyl ether	25	flammable
144	–25	1,2-dimethylbenzene	17	highly flammable
146	30	triethyl orthoformate	30	flammable
150	–51	nonane	30	flammable
153	–61	dimethylformamide	55	flammable
155	–38	methoxybenzene	52	flammable
155	–45	cyclohexanone	44	flammable
156	–31	bromobenzene	51	flammable
161	–68	diglyme	67	flammable
166	–20	*N*,*N*-dimethylacetamide	67	flammable
172	–75	2-butoxyethanol	61	flammable
175	–42	2,4,6-trimethylpyridine	57	flammable
180	–17	1,2-dichlorobenzene	66	flammable
185	–31	*trans*-decahydronaphthalene	54	flammable
189	18	dimethyl sulfoxide	95	
191	–13	benzonitrile	72	
195	–17	1-octanol	85	
196	–46	trimethyl phosphate	107	
196	–43	*cis*-decahydronaphthalene	54	flammable
197	–13	1,2-ethanediol	111	
202	20	acetophenone	77	
202	–2	▶hexachloro-2-propanone		non-flammable
202	–24	1-methyl-2-pyrrolidinone	96	
205	–15	benzyl alcohol	93	
207	<–50	1,3-butanediol	109	
207	–35	1,2,3,4-tetrahydronaphthalene	78	
210	3	formamide	>77	
211	6	▶nitrobenzene	88	
214	17	1,2,4-trichlorobenzene	105	
215	–12	dodecane	74	
216	–45	1,2-bis(2-methoxyethoxy)ethane	111	
222	82	acetamide	>104	
235	7	▶hexamethylphosphoric triamide	>55	
238	–16	▶quinoline	>55	
240	–55	4-methyl-1,3-dioxolan-2-one	135	
255	72	biphenyl	>55	
279	96	acenaphthene	>66	
285	27	tetrahydrothiophene 1,1-dioxide	177	
290	18	glycerol	160	
328	–6	tetraethylene glycol	174	

[a] ▶Solvent presenting severe potential toxic hazard.

[b] Solvents having flash points above 55°C are considered non-flammable, but may ignite if brought to a high temperature.

[c] Mixture of hydrocarbons, typically 73% *n*-pentane, 23% branched pentanes, 3% cyclopentane. Higher boiling petrols have correspondingly decreasing flammability hazards.

Organo-Chlorine Solvents: Health Risks to Workers, Royal Society of Chemistry, London, 1986.

Patty's Industrial Hygiene and Toxicology, 3rd & 4th edns, ed. G.D. Clayton, *et al.*, Wiley, Chichester, 1978 & 1991.

Riddick, J.A., *et al.*, *Organic Solvents: Physical Properties and Methods of Purification*, 4th edn, Wiley-Interscience, New York, 1986.

Solvents in Common Use: Health Risks to Workers, Royal Society of Chemistry, London, 1988.

16 Miscellaneous

16.1 Buffer solutions

A list of buffer solutions that show round values of pH at 25 °C is given in Table 16.1. The information has been obtained from Bower, V.E. and Bates, R.G., *J. Res. Natl. Bur. Stand.*, 1955, **55**, 197 (A–D), and Bates, R.G. and Bower, V.E., *Anal. Chem.*, 1956, **28**, 1322 (E–J). The final volume of all the mixtures is 100 ml.

16.2 Resolving agents

The following resolving agents are among those listed in DOC 6. The resolution of an organic compound in practice usually requires a wide range of trial and error. Key sources of information on resolution techniques include the following:

Stereochemistry, Fundamentals and Methods, ed. H.B. Kagan, vol. 3, Georg Thieme Verlag, 1977.

Thielheimer's Synthetic Methods of Organic Chemistry (this series lists resolutions on a separate index section since 1986).

16.2.1 Bases

2-amino-3-methyl-1-butanol
2-amino-1-(4-nitrophenyl)-1,3-propanediol
2-amino-1-phenyl-1-propanol (norephedrine, norpseudoephedrine)
2-amino-3-phenyl-1-propanol
N-isopropylphenylalaninol
brucine
cinchonidine
cinchonine
2,2′-diamino-1,1′-binaphthyl
2-methyl-2-phenylbutanedioic acid anhydride
1-(1-naphthyl)ethylamine
1-phenyl-1-propylamine
1-phenyl-2-propylamine
quinine
sparteine
strychnine
1,2,3,4-tetrahydro-3-isoquinolinesulfonic acid

Plus many suitable derivatives of the common protein amino acids.

16.2.2. Acids

(1,1′-binaphthalene)-2,2′-dicarboxylic acid
3-bromo-8-camphorsulfonic acid
camphor-8-sulfonic acid
camphor-10-sulfonic acid
7,7-dimethyl-2-oxobicyclo[2.2.1]heptane-1-carboxylic acid
2,3:4,6-di-*O*-isopropylidene-*xylo*-hexulosonic acid
4-hydroxydinaphtho[2,1-*d*:1′,2′-*f*]-1,3,2-dioxaphosphepin 4-oxide
4-hydroxy-3-phenylbutanoic acid lactone
Mosher's reagent
lactic acid and many of its derivatives
mandelic acid and many of its derivatives
3-menthoxyacetic acid
3-menthylglycine
2-methyl-2-phenylbutanedioic acid
naproxen
5-oxo-2-pyrrolidinecarboxylic acids
2-[((phenylamino)carbonyl)oxy]propanoic acid
1-phenylethanesulfonic acid
tartaric acid and many of its derivatives
1,2,3,4-tetrahydro-3-isoquinolinesulfonic acid
(2,4,5,7-tetranitro-9-fluorenylideneaminoxy)-propionic acid
4-thiazolidinecarboxylic acid

Plus many suitable derivatives of the common protein amino acids.

16.2.3 Others

camphor-10-sulfonyl chloride
chrysanthemic acid chloride
(1,1′-binaphthalene)-2,2′-diol
camphor

Table 16.1 Buffer solutions[a] giving round values of pH at 25°C

A		B		C		D		E	
pH	x	pH	x	pH	x	pH	x	pH	x
1.00	67.0	2.20	49.5	4.10	1.3	5.80	3.6	7.00	46.6
1.10	52.8	2.30	45.8	4.20	3.0	5.90	4.6	7.10	45.7
1.20	42.5	2.40	42.2	4.30	4.7	6.00	5.6	7.20	44.7
1.30	33.6	2.50	38.8	4.40	6.6	6.10	6.8	7.30	43.4
1.40	26.6	2.60	35.4	4.50	8.7	6.20	8.1	7.40	42.0
1.50	20.7	2.70	32.1	4.60	11.1	6.30	9.7	7.50	40.3
1.60	16.2	2.80	28.9	4.70	13.6	6.40	11.6	7.60	38.5
1.70	13.0	2.90	25.7	4.80	16.5	6.50	13.9	7.70	36.6
1.80	10.2	3.00	22.3	4.90	19.4	6.60	16.4	7.80	34.5
1.90	8.1	3.10	18.8	5.00	22.6	6.70	19.3	7.90	32.0
2.00	6.5	3.20	15.7	5.10	25.5	6.80	22.4	8.00	29.2
2.10	5.1	3.30	12.9	5.20	28.8	6.90	25.9	8.10	26.2
2.20	3.9	3.40	10.4	5.30	31.6	7.00	29.1	8.20	22.9
		3.50	8.2	5.40	34.1	7.10	32.1	8.30	19.9
		3.60	6.3	5.50	36.6	7.20	34.7	8.40	17.2
		3.70	4.5	5.60	38.8	7.30	37.0	8.50	14.7
		3.80	2.9	5.70	40.6	7.40	39.1	8.60	12.2
		3.90	1.4	5.80	42.3	7.50	40.9	8.70	10.3
		4.00	0.1	5.90	43.7	7.60	42.4	8.80	8.5
						7.70	43.5	8.90	7.0
						7.80	44.5	9.00	5.7
						7.90	45.3		
						8.00	46.1		

F		G		H		I		J	
pH	x	pH	x	pH	x	pH	x	pH	x
8.00	20.5	9.20	0.9	9.60	5.0	10.90	3.3	12.00	6.0
8.10	19.7	9.30	3.6	9.70	6.2	11.00	4.1	12.10	8.0
8.20	18.8	9.40	6.2	9.80	7.6	11.10	5.1	12.20	10.2
8.30	17.7	9.50	8.8	9.90	9.1	11.20	6.3	12.30	12.8
8.40	16.6	9.60	11.1	10.00	10.7	11.30	7.6	12.40	16.2
8.50	15.2	9.70	13.1	10.10	12.2	11.40	9.1	12.50	20.4
8.60	13.5	9.80	15.0	10.20	13.8	11.50	11.1	12.60	25.6
8.70	11.6	9.90	16.7	10.30	15.2	11.60	13.5	12.70	32.2
8.80	9.6	10.00	18.3	10.40	16.5	11.70	16.2	12.80	41.2
8.90	7.1	10.10	19.5	10.50	17.8	11.80	19.4	12.90	53.0
9.00	4.6	10.20	20.5	10.60	19.1	11.90	23.0	13.00	66.0
9.10	2.0	10.30	21.3	10.70	20.2	12.00	26.9		
		10.40	22.1	10.80	21.2				
		10.50	22.7	10.90	22.0				
		10.60	23.3	11.00	22.7				
		10.70	23.8						
		10.80	24.25						

[a] The buffer solutions are made up as follows:
(A) 25 ml of 0.2 molar KCl + x ml of 0.2 molar HCl.
(B) 50 ml of 0.1 molar potassium hydrogen phthalate + x ml of 0.1 molar HCl.
(C) 50 ml of 0.1 molar potassium hydrogen phthalate + x ml of 0.1 molar NaOH.
(D) 50 ml of 0.1 molar potassium dihydrogen phosphate + x ml of 0.1 molar NaOH.
(E) 50 ml of 0.1 molar tris(hydroxymethyl) aminomethane + x ml of 0.1 molar HCl.
(F) 50 ml of 0.025 molar borax + x ml of 0.1 molar HCl.
(G) 50 ml of 0.025 molar borax + x ml of 0.1 molar NaOH.
(H) 50 ml of 0.05 molar sodium bicarbonate + x ml of 0.1 molar NaOH.
(I) 50 ml of 0.05 molar disodium hydrogen phosphate + x ml of 0.1 molar NaOH.
(J) 25 ml of 0.2 molar KCl + x ml of 0.2 molar NaOH.
A–D reproduced with permission from V.E. Bower and R.G. Bates, *J. Res. Natl. Bur. Stasnd.*, **55**, 197; copyright by the American Geophysical Union, 1955.
E–J reprinted with permission from R.G. Bates and V.E. Bower, *Anal. Chem.*, **28**, 1322. Copyright 1956

2,2′-dimethoxybutanedioic acid bis(dimethylamide)
3,3-dimethyl-2-butanol
7,7-dimethyl-2-oxobicyclo[2.2.1]heptane-1-carbonyl chloride
2,2-dimethyl-α,α,α′,α′-tetraphenyl-1,3-dioxolane-4,5-dimethanol
α-methoxy-α-(trifluoromethyl)benzene acetic acid chloride
1-(1-isocyanatoethyl)naphthalene
menthol and its stereoisomers
3-menthoxyacetyl chloride
N-methanesulfonylphenylalanyl chloride
methyl phenyl sulfoximine

Table 16.2 Solvents commonly used for recrystallisation[a]. Solvents are listed in approximate order of decreasing polarity

Solvent	Bp (°C)	Mp (°C)	Flash point (°C)	Good for	Second solvent for mixture
water	100	0	none	salts, amides, carboxylic acids	acetone, ethanol, methanol, dioxane
methanol	65	–98	10	many compounds	water, diethyl ether, dichloromethane, benzene
ethanol	78	–117	12	many compounds	water, petrol, pentane, hexane, ethyl acetate
acetone	56	–94	–17	many compounds	water, petrol, pentane, hexane, diethyl ether
2-methoxyethanol	125	–86	43	sugars	water, benzene, diethyl ether
pyridine	116	–42	20	high-melting compounds	water, methanol, petrol, pentane, hexane
dichloromethane	40	–97	none	low-melting compounds	ethanol, methanol, petrol, pentane, hexane
methyl acetate	56	–98	–9	many compounds	water, diethyl ether
acetic acid	118	+17	39	salts, amides, carboxylic acids	water, diethyl ether
ethyl acetate	77	–84	–4	many compounds	diethyl ether, benzene, petrol, pentane, hexane
chloroform	61	–63	none	many compounds	ethanol, petrol, pentane, hexane
diethyl ether	35	–116	–45	low-melting compounds	acetone, methanol, ethanol, petrol, pentane, hexane
1,4-dioxane	101	+11	11	amides	water, benzene, petrol, pentane, hexane
tetrachloromethane	77	–21	none	non-polar compounds	diethyl ether, benzene, petrol, pentane, hexane
toluene	111	–95	4	aromatics, hydrocarbons	diethyl ether, ethyl acetate, petrol, pentane, hexane
benzene	80	+6	–11	aromatics, hydrocarbons	diethyl ether, ethyl acetate, petrol, pentane, hexane
petrol	–[b]	–[b]	–40	hydrocarbons	most solvents
pentane	36	–129	–49	hydrocarbons	most solvents
hexane	69	–94	–23	hydrocarbons	most solvents

[a] This table is based on that in *The Chemist's Companion*, A.J. Gordon and R.A. Ford, Wiley–Interscience, New York, 1972. For further information on these solvents see *Organic Solvents: Physical Properties and Methods of Purification*, 4th edn, J.A. Riddick, *et al.*, Wiley, Chichester, 1986.

[b] Petrol refers to a mixture of alkanes obtainable in a number of grades based on boiling ranges, e.g. 40–60°C and 60–80°C.

2-phenylpropanoic acid chloride
tri-*O*-thymoltide

16.3 Solvents for recrystallisation

A solid is purified by recrystallisation by dissolving it in a minimum of hot solvent, filtering the solution, and then cooling the solution so that crystals of the desired substance form while the impurities remain in solution.

A list of solvents used for recrystallisation is given in Table 16.2. In order to be useful, a solvent should dissolve a great deal of the solid substance at high temperatures and very little of it at low temperatures. It should not react with the compound. Solvents with a high boiling point should be avoided if possible. It should be noted that the impurities do not have to be more soluble in the cold solvent than the substance being purified. Since the impurities are present at a lower concentration, they will frequently remain in solution even though less soluble.

Normally polar compounds (e.g. alcohols, thiols, amines, carboxylic acids, amides) tend to dissolve in polar solvents (e.g. water, alcohols). Non-polar compounds tend to dissolve in non-polar solvents (e.g. benzene, petrol, hexane).

Often it is possible to use a mixture of miscible solvents where the substance to be recrystallised is soluble in one of the solvents but relatively insoluble in the other. The solute can be dissolved hot in a suitable solvent mixture, which is then allowed to cool; alternatively, the solute can be dissolved hot in the solvent in which it is more soluble, the other solvent added until crystallization just begins, and the resulting mixture allowed to cool slowly.

16.4 Materials used for heating baths

A list of materials that can be used for heating baths is given in Table 16.3.

16.5 Freezing mixtures

Table 16.4 presents a list of freezing mixtures and their approximate temperatures.

16.6 Solvents for extraction of aqueous solutions

A list of solvents that can be used for the extraction of aqueous solutions is given in Table 16.5. For further information about these solvents, including hazard and toxicity data, see Section 15.1.

Table 16.3 Heating baths

Medium	Mp (°C)	Bp (°C)	Useful range (°C)	Flash point (°C)	Comments
water	0	100	0–100	none	ideal
silicone oil	–50	–	30–250	~300	becomes viscous at low temperature
triethylene glycol	–5	285	0–250	165	water-soluble, stable
glycerol	18	290	–20 to 260	160	water-soluble, non toxic, viscous, supercools
paraffin	~50	–	60–300	199	flammable
dibutyl phthalate	–35	340	150–320	171	viscous at low temperature
sand	–	–	>about 200	none	ideal for high temperature heating
Wood's metal	70	–	73–350	none	ideal for high temperature heating

Table 16.4 Freezing mixtures

Components		Approximate temperature (°C)
100 g water	100 g ice	0
100 g water	30 g ammonium chloride	–3
100 g water	75 g sodium nitrate	–5
100 g water	85 g sodium acetate	–5
100 g water	110 g sodium thiosulfate	–8
100 g water	36 g sodium chloride	–10
100 g water	245 g calcium chloride hexahydrate	–12
100 g water	133 g ammonium thiocyanate	–16
100 g ice	45 g ammonium nitrate	–17
100 g ice	30 g sodium chloride	–21
100 g ice	81 g calcium chloride hexahydrate	–21
100 g ice	66 g sodium bromide	–28
100 g ice	85 g magnesium chloride	–34
100 g powdered ice	92 g 66.1% sulfuric acid	–37
100 g ice	123 g calcium chloride hexahydrate	–40
100 g ice	143 g calcium chloride hexahydrate	–55
ethanol	carbon dioxide (solid)	–72
chloroform	carbon dioxide (solid)	–77
acetone	carbon dioxide (solid)	–86
ether	carbon dioxide (solid)	–100

Table 16.5 Solvents for extracting aqueous solutions

Solvent	Bp (°C)	Density relative to water	Flash point (°C)	Solubility of solvent in water (wt%)	Solubility of water in solvent (wt%)	Comments
benzene	80	lighter	–11	0.18	0.06	tends to form emulsions
2-butanol	99	lighter	31	12.5	44.1	dries easily; good for highly polar water-soluble materials from buffered solution
tetrachloromethane	77	heavier	none	0.08	0.01	dries easily; good for non-polar materials
chloroform	61	heavier	none	0.82	0.09	may form emulsions; dries easily
diethyl ether	35	lighter	–40	6.04	1.47	absorbs large amounts of water
diisopropyl ether	69	lighter	–12	1.2	0.57	tends to form peroxide on storage
ethyl acetate	77	lighter	–3	8.08	2.94	absorbs large amounts of water; good for polar materials
dichloromethane	40	heavier	none	1.30	0.02	may form emulsions; dries easily
pentane	36	lighter	–49	0.004	0.01	dries easily
hexane	69	lighter	–23	0.002	0.01	dries easily

16.7 Drying agents

Table 16.6 presents a list of drying agents along with their uses and some comments on their use.

16.8 Pressure–temperature nomograph

A pressure–temperature nomograph for correcting boiling points to 760 mmHg (1 atm) is shown in Figure 16.1 (this can be found in the Aldrich catalogue, the Lancaster catalogue, etc.). It is used as follows: If the boiling point at non-atmospheric pressure (P mmHg) is known, line up the values of the boiling point in **A** and the pressure in **C**. The theoretical boiling point at 760 mmHg can then be read off in **B**. Line up this figure in **B** with another pressure in **C** and the approximate corresponding boiling point can be read off in **A**.

Table 16.6 Drying agents

Drying agent	Useful for	Comments
alumina (Al_2O_3)	hydrocarbons	very high capacity; very fast; reactivated by heating
barium oxide (BaO)	hydrocarbons, amines, alcohols, aldehydes	slow but efficient; not suitable for compounds sensitive to strong base
calcium chloride ($CaCl_2$)	hydrocarbons, alkyl halides, ethers, many esters	not very efficient; good for pre-drying; not suitable for most nitrogen and oxygen compounds
calcium hydride (CaH_2)	hydrocarbons, ethers, amines, esters, higher alcohols (> C_4)	not suitable for aldehydes and ketones
calcium oxide (CaO)	low-boiling alcohols and amines, ethers	slow but efficient; not suitable for acidic compounds
calcium sulfate ($CaSO_4$)	most organic substances	very fast and very efficient
lithium aluminium hydride ($LiAlH_4$)	hydrocarbons, aryl halides, ethers	excess may be destroyed by slow addition of ethyl acetate; pre-drying recommended; reacts with acidic hydrogens and most functional groups
magnesium sulfate ($MgSO_4$)	most organic substances	very fast and very efficient; avoid using with very acid-sensitive compounds
molecular sieves 4 Å	non-polar liquids and gases	very efficient; pre-drying with a common agent recommended; can be reactivated by heating
phosphorus pentoxide (P_2O_5)	hydrocarbons, ethers, halides, esters, nitriles	fast and efficient; pre-drying recommended; most suitable for alcohols, amines, acids, ketones, etc.
potassium carbonate (K_2CO_3)	alcohols, esters, nitriles, ketones	not suitable for acidic compounds
potassium hydroxide (KOH)	amines (in inert solvents)	powerful; not suitable for acidic compounds
silica gel	hydrocarbons, amines	very high capacity and very fast; can be reactivated by heating
sodium (as 9.5% Na–Pb alloy)	saturated and aromatic hydrocarbons, ethers	not suitable for halides, alcohols, amines, esters, etc.
sodium sulfate (Na_2SO_4)	most organic substances	inefficient and slow; good for gross pre-drying
sulfuric acid (H_2SO_4)	saturated and aromatic hydrocarbons, halides, inert neutral or acidic gases	very high capacity; very fast

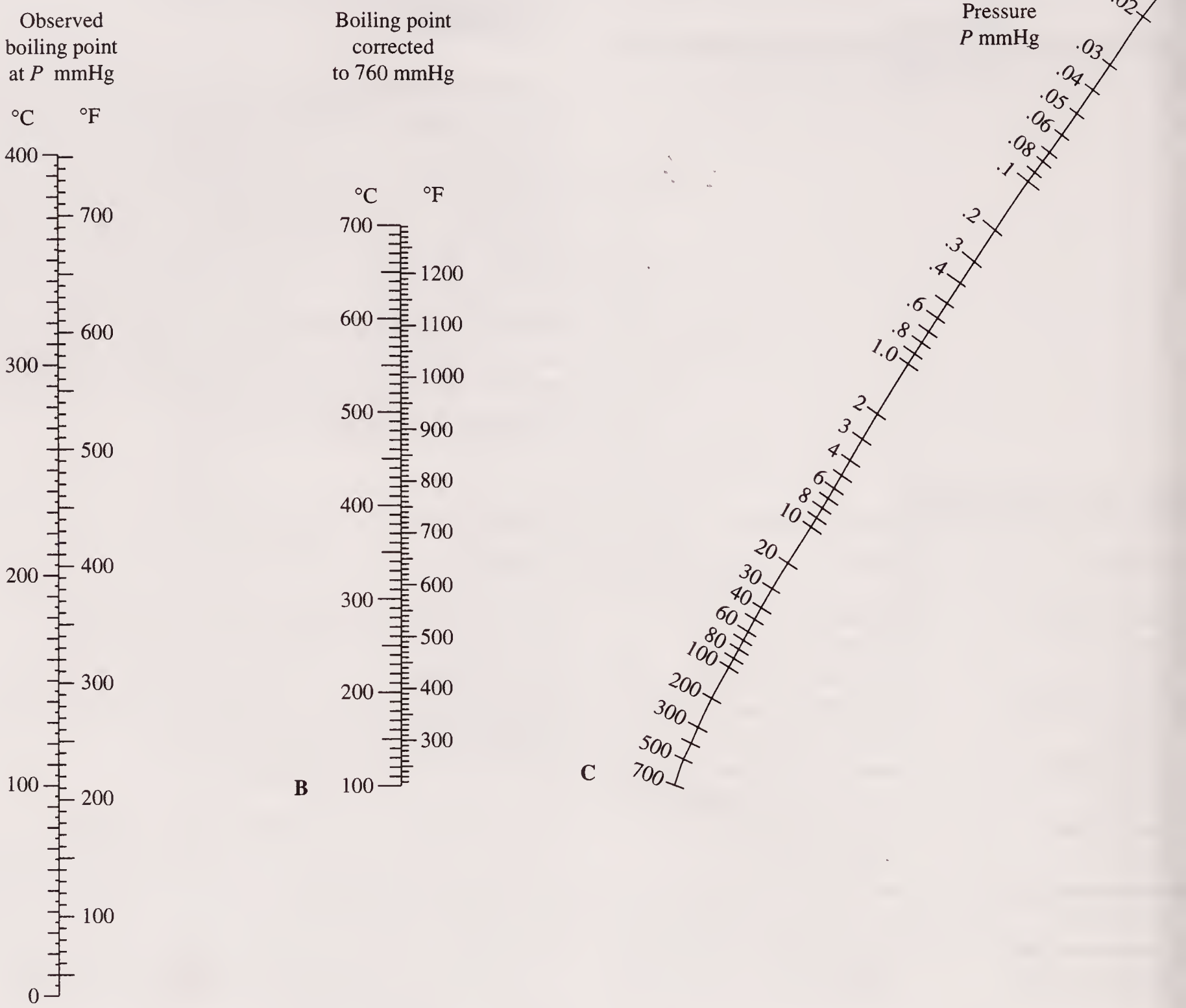


Figure 16.1 Pressure–temperature nomograph.

16.9 Acid and base dissociation constants

16.9.1 First dissociation constants of organic acids in aqueous solution at 298 K

Some pK_{a1} values are listed in Table 16.7.

Table 16.7 The pK_{a1} values of some organic acids in aqueous solution at 298 K

pK_{a1}	Compound (DOC Name)	pK_{a1}	Compound (DOC Name)
0.17	1-naphthalenesulfonic acid	3.70	1-naphthalenecarboxylic acid
0.29	2,4,6-trinitrophenol	3.74	formic acid
0.66	trichloroacetic acid	3.83	hydroxyacetic acid
0.70	benzenesulfonic acid	3.86	2-hydroxypropanoic acid
1.10	nitrilotriacetic acid	3.91	2-methylbenzoic acid
1.25	oxalic acid	4.01	2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione
1.48	dichloroacetic acid	4.08	3-hydroxybenzoic acid
1.70	histidine	4.09	2,4-dinitrophenol
1.71	cysteine	4.16	succinic acid
1.75	2-butynedioic acid	4.17	2-naphthalenecarboxylic acid
1.82	arginine	4.20	benzoic acid
1.83	maleic acid	4.26	2-propenoic acid
1.95	proline	4.27	3-methylbenzoic acid
1.99	aspartic acid (α-COOH)	4.30	ascorbic acid
2.04	lysine	4.31	phenylacetic acid
2.09	threonine	4.34	pentanedioic acid
2.14	asparagine	4.36	4-methylbenzoic acid
2.17	glutamine	4.43	hexanedioic acid
2.17	tyrosine	4.44	3-phenyl-2-propenoic acid (*E*-)
2.17	2-nitrobenzoic acid	4.48	heptanedioic acid
2.19	serine	4.58	4-hydroxybenzoic acid
2.20	methionine	4.69	2-butenoic acid (*E*-)
2.23	glutamic acid (α-COOH)	4.78	acetic acid
2.23	fluoroacetic acid	4.78	3-methylbutanoic acid
2.29	valine	4.78	3-aminobenzoic acid
2.32	isoleucine	4.83	butanoic acid
2.32	leucine	4.84	pentanoic acid
2.35	glycine	4.84	2-methylpropanoic acid
2.35	tryptophan	4.85	3-pyridinecarboxylic acid
2.35	alanine	4.87	propanoic acid
2.49	pyruvic acid	4.88	hexanoic acid
2.69	bromoacetic acid	4.89	octanoic acid
2.85	propanedioic acid	4.92	4-aminobenzoic acid
2.86	chloroacetic acid	4.96	4-pyridinecarboxylic acid
2.89	1,2-benzenedioic acid	5.03	2,2-dimethylpropanoic acid
2.95	phosphoric acid	5.22	3,6-dinitrophenol
2.97	2-hydroxybenzoic acid	5.52	2-pyridine carboxylic acid
2.98	tartaric acid ((±)-)	8.49	2-chlorophenol
3.05	fumaric acid	8.85	3-chlorophenol
3.12	iodoacetic acid	9.12	1,2-benzenediol
3.13	citric acid	9.15	1,3-benzenediol
3.17	2-furancarboxylic acid	9.18	4-chlorophenol
3.22	tartaric acid (*meso*-)	9.34	1-naphthol
3.23	2-aminobenzoic acid	9.51	2-naphthol
3.33	ethanethioic acid	9.91	1,4-benzenediol
3.40	hydroxybutanedioic acid	9.99	phenol
3.44	4-nitrobenzoic acid	10.01	3-methylphenol
3.46	glyoxylic acid	10.17	4-methylphenol
3.49	3-nitrobenzoic acid	10.20	2-methylphenol
3.51	1,4-benzenedicarboxylic acid	14.15	glycerol
3.54	1,3-benzenedicarboxylic acid	14.22	1,2-ethanediol
3.60	mercaptoacetic acid		

16.9.2 Dissociation constants of organic bases in aqueous solution at 298 K

Some pK_a values are listed in Table 16.8. The dissociation constant of a base B is given in terms of the pK_a value of its conjugate acid BH^+. The pK_b of a base may be calculated from the pK_a value of its conjugate acid using the equation

$$pK_b = pK_w - pK_a$$

at 298 K, this becomes

$$pK_b = 14.00 - pK_a$$

Table 16.8 The pK_a values of some organic acids in aqueous solution at 298 K

pK_a	Compound (DOC Name)	pK_a	Compound (DOC Name)
0.10	urea	5.68	3-methylpyridine
0.60	1,2-benzenediamine	5.96	hydroxylamine
0.63	acetamide	5.97	2-methylpyridine
0.65	pyrazine	6.02	4-methylpyridine
0.79	diphenylamine	6.15	3,5-dimethylpyridine
1.00	4-nitroaniline	6.57	2,3-dimethylpyridine
2.24	pyridazine	6.61	1,2-propanediamine
2.30	1,3-benzenediamine	6.82	2-aminopyridine
2.30	purine	6.85	1,2-ethanediamine
2.44	thiazole	6.99	2,4-dimethylpyridine
2.47	3-nitroaniline	6.99	imidazole
2.48	pyrazole	7.76	tris(2-hydroxyethyl)amine
2.61	*N*,*N*-diethylaniline	8.01	2-amino-2-hydroxymethyl-1,3-propanediol
2.65	2-chloroaniline	8.28	brucine
2.70	1,4-benzenediamine	8.49	morpholine
3.12	nicotine	8.88	diethanolamine
3.52	3-chloroaniline	9.03	1,3-propanediamine
3.92	1-naphthalenamine	9.11	4-aminopyridine
4.05	pteridine	9.35	benzylamine
4.12	adenine	9.50	2-aminoethanol
4.13	quinine	9.80	trimethylamine
4.14	4-chloroaniline	10.41	2-methylpropylamine
4.16	2-naphthalenamine	10.56	2-butylamine
4.35	2,2′-bipyridine	10.56	hexylamine
4.45	2-methylaniline	10.60	2-propylamine
4.60	aniline	10.61	butylamine
4.66	4,4′-biphenyldiamine	10.64	decylamine
4.73	3-methylaniline	10.64	cyclohexylamine
4.78	2-aminophenol	10.64	ethylamine
4.85	*N*-methylaniline	10.64	methylamine
4.86	1,10-phenanthroline	10.71	propylamine
4.88	quinoline	10.72	triethylamine
4.91	8-hydroxyquinoline	10.77	dimethylamine
5.08	4-methylaniline	10.83	*tert*-butylamine
5.12	*N*-ethylaniline	10.93	diethylamine
5.15	*N*,*N*-dimethylaniline	11.12	piperidine
5.23	pyridine	11.30	pyrrolidine
5.33	piperazine	12.34	1,8-bis(dimethylamino)naphthalene
5.42	isoquinoline	13.54	guanidine
5.58	acridine		

17 Spectroscopy

The regions of the electromagnetic spectrum are shown in Table 17.1. The following four sections deal with infrared (ir) spectroscopy, ultraviolet (uv) spectroscopy, nuclear magnetic resonance (nmr) and mass spectrometry, respectively.

Table 17.1 The electromagnetic spectrum

Region	Range
Vacuum ultraviolet	100–180 nm
Ultraviolet	180–400 nm
Visible	400–750 nm
Near-infrared	0.75–2.5 μm
Infrared	2.5–15 μm
Far-infrared	15–300 μm

17.1 Infrared spectroscopy

17.1.1 Window materials, mulling oils and solvents

(*a*) Window materials

The transmission ranges of various window materials are listed in Table 17.2.

Table 17.2 Window materials

Material	Transmission range (cm^{-1})
NaCl	40 000–590
KBr	40 000–400
AgCl	25 000–435
CaF_2	67 000–1100
CsBr	10 000–270
ZnS	10 000–680

(*b*) Mulling oils

Nujol® (a high-molecular-weight hydrocarbon) can be used from 1370 cm^{-1} to the far-infrared. It gives ir signals around 2900 (vs), 1460 and 1350 cm^{-1}. Fluorolube® (a high-molecular-weight fluorinated hydrocarbon) is useful for the range 4000 to 1370 cm^{-1}.

(*c*) Solvents

The following solvents are commonly used to record ir spectra. They *cannot* be used in the regions shown (cm^{-1}).

- Carbon disulfide
  - 1 mm cell 2340–2100, 1640–1385, 875–845
  - 0.1 mm cell 2200–2140, 1595–1460
- Carbon tetrachloride
  - 1 mm cell 1610–1500, 1270–1200, 1020–960, < 860
  - 0.1 mm cell 820–720
- Chloroform
  - 1 mm cell 3090–2980, 2440–2380, 1555–1410, 1290–1155, 940–910, < 860
  - 0.1 mm cell 3020–3000, 1240–1200, < 805

17.1.2 Characteristic infrared absorption bands

The characteristic ir absorption bands of various types of compounds are listed in Table 17.3, in two complementary formats.

17.2 Ultraviolet spectroscopy

17.2.1 Ultraviolet cut-off limits for solvents

These cut-off limits, which are listed in Table 17.4, are the wavelengths at which the absorbance approaches 1.0 in a 10 mm cell.

Table 17.3 Characteristic ir absorption bands

(a) Presented alphabetically by type of compound

Type of compound	Bond	Type of vibration	Frequency (cm^{-1})
alcohols	C–O	stretching	1300–1050
(not H-bonded)	O–H	stretching	3650–3600
(H-bonded)	O–H	stretching	3600–3200
aldehydes	C–H	stretching	2900–2700
	C=O	stretching	1740–1690
alkanes	C–H	stretching	3000–2800
alkenes	C=C	stretching	1680–1600
	C–H	bending	975–675
	C–H	stretching	3100–3000
alkyl bromides	C–Br	stretching	680–500
chlorides	C–Cl	stretching	850–600
fluorides	C–F	stretching	1400–1000
iodides	C–I	stretching	500–200
alkynes	C–H	stretching	3350–3300
	C≡C	stretching	2250–2100
amides	C=O	stretching	1715–1630
amines	N–H	bending	1650–1550
	C–H	stretching	1350–1000
	N–H	stretching	3500–3100
aromatics	C–H	bending	900–680
	C–H	stretching	3150–3000
carboxylic acids	O–H	stretching	3400–2400
	C=O	stretching	1750–1690
	C–O	stretching	1300–1080
esters	C–O	stretching	1300–1080
	C=O	stretching	1750–1730
ethers	C–O	stretching	1300–1080
imines/oximes	C=N	stretching	1690–1640
ketones	C=O	stretching	1730–1650
nitriles	C≡N	stretching	2260–2240
phosphorus compounds	P=O	stretching	1300–960
	P–O	stretching	1260–855
	P–H	bending	1090–910
thiols	S–H	stretching	2600–2500

Table 17.3 *Continued*

(b) Presented in order of decreasing frequency

Type of compound	Bond	Type of vibration	Frequency (cm^{-1})
alcohols	O–H	stretching	3650–3600
alcohols	O–H	stretching	3600–3200
amines	N–H	stretching	3500–3100
carboxylic acids	O–H	stretching	3400–2400
alkynes	C–H	stretching	3350–3300
aromatics	C–H	stretching	3150–3000
alkenes	C–H	stretching	3100–3000
alkanes	C–H	stretching	3000–2800
aldehydes	C–H	stretching	2900–2700
thiols	S–H	stretching	2600–2500
nitriles	C≡N	stretching	2260–2240
alkynes	C≡C	stretching	2250–2100
esters	C=O	stretching	1750–1730
carboxylic acids	C=O	stretching	1750–1690
aldehydes	C=O	stretching	1740–1690
ketones	C=O	stretching	1730–1650
amides	C=O	stretching	1715–1630
imines/oximes	C=N	stretching	1690–1640
alkenes	C=C	stretching	1680–1600
amines	N–H	bending	1650–1550
alkyl fluorides	C–F	stretching	1400–1000
amines	C–N	stretching	1350–1000
carboxylic acids	C–O	stretching	1300–1080
esters	C–O	stretching	1300–1080
ethers	C–O	stretching	1300–1080
alcohols	C–O	stretching	1300–1050
phosphorus compounds	P=O	stretching	1300–960
phosphorus compounds	P–O	stretching	1260–855
phosphorus compounds	P–H	bending	1090–910
alkenes	C–H	bending	975–675
aromatics	C–H	bending	900–680
alkyl chlorides	C–Cl	stretching	850–600
alkyl bromides	C–Br	stretching	680–500
alkyl iodides	C–I	stretching	500–200

Table 17.4 Uv cut-off limits for solvents

Solvent	Wavelength (nm)
acetonitrile	190
water	205
methanol	210
cyclohexane	210
hexane	210
ethanol (95%)	210
1,4-dioxane	215
diethyl ether	215
tetrahydrofuran	220
dichloromethane	235
chloroform	245
carbon tetrachloride	265
benzene	280
toluene	285
acetone	330

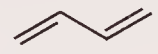
17.2.2 Characteristic ultraviolet/visible absorption bands

The characteristic uv/vis absorption bands for some representative chromophores are listed in Table 17.5.

17.2.3 Uv/vis absorption of dienes and polyenes

The Fieser–Woodward rules can be used to estimate the uv/vis absorption as follows:

Parent diene system

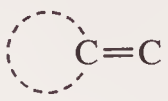


Acyclic 215 nm

Heteroannular 214 nm

Homoannular 253 nm

Increments

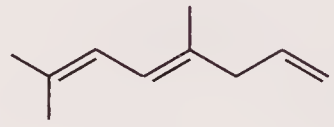
For each additional conjugated double bond	+30 nm
For each exocyclic double bond 	+5 nm

For each substituent

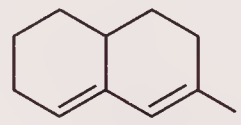
C substituent	+5 nm
OAc	0 nm
OR (R = alkyl)	+6 nm
SR (R = alkyl)	+30 nm
Cl, Br	+5 nm
NR_2 (R = alkyl)	+60 nm

Solvent correction 0 nm

Examples



acyclic	215 nm
four alkyl substituents	20 nm
	235 nm

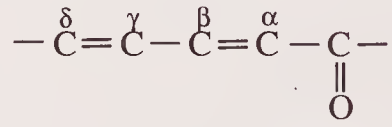


heteroannular	214 nm
four alkyl substituents	20 nm
exocyclic double bond	5 nm
	239 nm

17.2.4 Uv/vis absorption of α,β-unsaturated carbonyl compounds

The Woodward–Fieser rules can be used to estimate the uv/vis absorption as follows:

Parent system



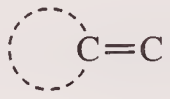
Acyclic α,β-unsaturated ketone	215 nm
α,β-Unsaturated aldehyde	207 nm
α,β-Unsaturated carboxylic acid or ester	193 nm
Six-membered cyclic α,β-unsaturated ketone	215 nm
Five-membered cyclic α,β-unsaturated ketone	202 nm

Increments

For each additional conjugated double bond	+30 nm

Table 17.5 Uv/vis absorption bands for representative chromophores

Chromophore		λ_{max} (ε_{max})
aldehydes	–CHO	180–210 (10 000), 280–300 (15)
amides	$-CONH_2$	175–180 (7000), 210–220) (60)
amines	$-NH_2$	190–200 (3000)
azides	$-N_3$	287 (20)
azo compounds	–N=N–	330–400 (10)
bromides	–Br	200–210 (300)
carboxylic acids	–COOH	195–210 (50)
chlorides	–Cl	170–175 (300)
disulfides	–S–S–	194 (5500), 250–255 (400)
esters	–COOR	195–210 (50)
ethers	–O–	180–185 (2000)
imines	>C=N–	190 (5000)
iodides	–I	255–260 (400)
ketones	>C=O	180–195 (1000), 270–290 (20)
nitriles	–C≡N	160–165 (5)
nitro compounds	$-NO_2$	200–210 (10 000), 275 (20)
nitroso compounds	–N=O	300 (100), 600–665 (20)
oximes	=N–OH	190–195 (5000)
sulfides	–S–	194 (4600), 210–215 (1500)
sulfones	$-SO_2-$	180
sulfoxides	–S(O)–	210–230 (1500)
thiols	–SH	190–200 (1500)
Unsaturated systems		
alkenes	–C=C–	162–175 (15 000), 190–195 (10 000)
alkynes	–C≡C–	175–180 (10 000), 195 (2000), 223 (150)
allenes	C=C=C	170–185 (5000), 225–230 (600)
ketenes	C=C=O	225–230 (600), 375–380 (20)
Conjugated systems (see Section 17.2.3 for Woodward–Fieser rules)		
$-(C=C)_2-$ (acyclic)		210–230 (21 000)
$-(C=C)_3-$		260 (35 000)
$-(C=C)_4-$		300 (52 000)
$-(C=C)_5-$		330 (118 000)
$-(C=C)_2-$ (cyclic)		230–260 (3000–8000)
–C=C–C≡C–		219–230 (7500)
–C=C–C=N–		220 (23 000)
–C=C–C=O		210–250 (10 000–20 000), 300–350 (30)
$-C=C-NO_2$		229–235 (9500)
–C≡C–C=O		214 (4500), 308 (20)
–C=C–COOH		206 (13 500), 242 (250)
–C≡C–COOH		210 (6000)
–C=C–C≡N		215 (680)
–C(O)C(O)–		195 (25), 280–285 (20), 420–460 (10)
Aromatic systems		
benzene		184 (46 700), 204 (6900), 255 (170)
biphenyl		246 (20 000)
naphthalene		222 (112 000), 275 (5600), 312 (175)
anthracene		252 (199 000), 375 (7900)
pyridine		174 (80 000), 195 (6000), 257 (1700)
quinoline		227 (37 000), 270 (3600), 314 (2750)
isoquinoline		218 (80 000), 266 (4000), 317 (3500)

For each
exocyclic double bond  +5 nm

For each
homoannular diene system  +39 nm

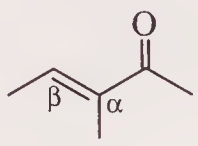
For each substituent at the π-electron system

	α	β	γ	δ and beyond
C substituent	10	12	18	18 nm
OH	35	30		50 nm
OAc	6	6	6	6 nm
OR (R = alkyl)	35	30	17	31 nm
SR (R = alkyl)		85 nm		
Cl	12	12 nm		
Br	25	30 nm		
NR_2 (R = alkyl)		95 nm		

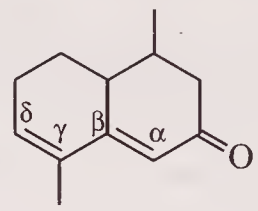
Solvent corrections

water	+8 nm
ethanol, methanol	0 nm
chloroform	–1 nm
dioxane	–5 nm
diethyl ether	–7 nm
hexane, cyclohexane	–11 nm

Examples



acyclic ketone	215 nm
α-alkyl group	10 nm
β-alkyl group	12 nm
	237 nm



six-membd. cyclic ketone	215 nm
addnl. conjugated bond	+30 nm
exocyclic bond	+5 nm
β-alkyl group	+12 nm
γ-alkyl group	+18 nm
δ-alkyl group	+18 nm
	298 nm

17.3 Nuclear magnetic resonance

17.3.1 Common nuclei used in nmr

These are listed in Table 17.6, along with details on nmr frequency and isotopic abundance.

17.3.2 Chemical shifts

Table 17.7 contains a summary of chemical shift values for the solvents that are used in nmr spectroscopy. The ranges of the ^{1}H, ^{13}C, ^{19}F and ^{31}P nmr chemical shifts of various groups are shown in Figures 17.1 to 17.4, respectively.

Table 17.6 Common nuclei used in nmr

Nucleus	Spin	Nmr frequency (Hz) at 14.092 G	Nmr frequency (Hz) at 23.49 G	Isotopic abundance (%)
^{1}H	1/2	60.0	100.0	99.98
^{2}H	1	9.2	15.3	0.01
^{11}B	3/2	19.2	32.1	80.42
^{13}C	1/2	15.1	25.1	1.11
^{14}N	1	4.3	7.2	99.63
^{15}N	(–)1/2	6.1	10.1	0.37
^{17}O	(–)5/2	8.1	13.6	0.037
^{19}F	1/2	56.5	94.1	100
^{31}P	1/2	24.3	40.5	100

Table 17.7 Chemical shifts for solvents used in nmr

Solvent	Formula	δ for residual protons (ppm)	δ ^{13}C (ppm)
acetic acid-d_4	D_3CCOOD	2.0, 11.5[a]	21, 177
acetone-d_6	$(D_3C)_2CO$	2.0	30, 205
acetonitrile-d_3	D_3CCN	2.0	0.3, 117
benzene-d_6	C_6D_6	7.2	128
carbon disulfide	CS_2		1931
carbon tetrachloride	CCl_4		97
chloroform-d	$CDCl_3$	7.3	77
deuterium oxide	D_2O	4.8[a]	
dimethyl-d_6 sulfoxide	$(D_3C)_2SO$	2.5	43
1,4-dioxane		3.7	67
methanol-d_4	D_3COD	3.4, 4.8[a]	49
hexachloroacetone	$(Cl_3C)_2CO$		124, 126
pyridine-d_5	C_5D_5N	7.2, 7.6, 8.5	124–150
toluene-d_8	$C_6D_5CD_3$	2.4, 7.3	21, 125–138
trifluoroacetic acid-d	F_3CCOOD	13.0	115, 163

[a] Value may vary considerably depending on the solute.

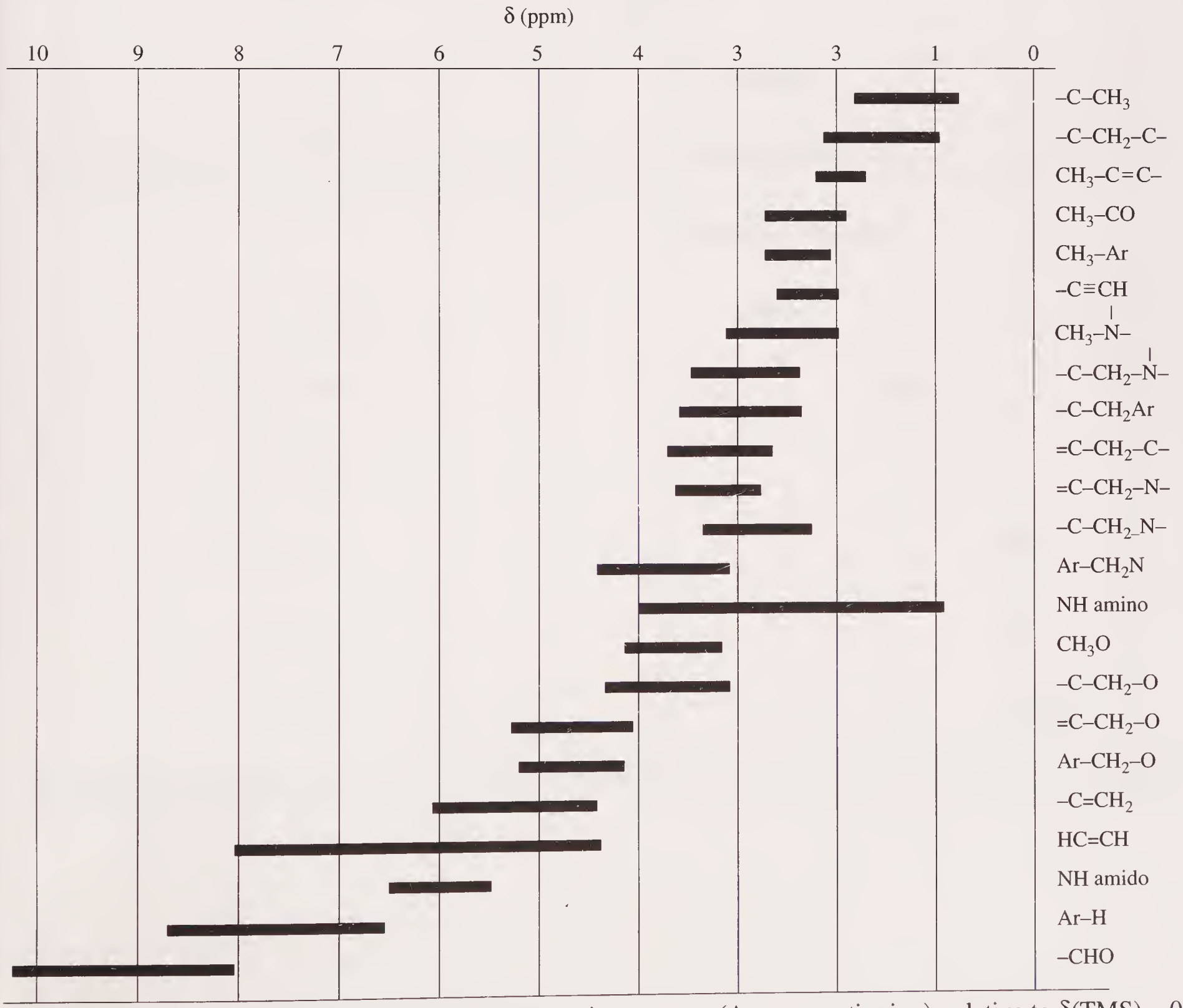


Figure 17.1 Ranges of ^1H nmr chemical shifts for various groups (Ar = aromatic ring), relative to δ(TMS) = 0.

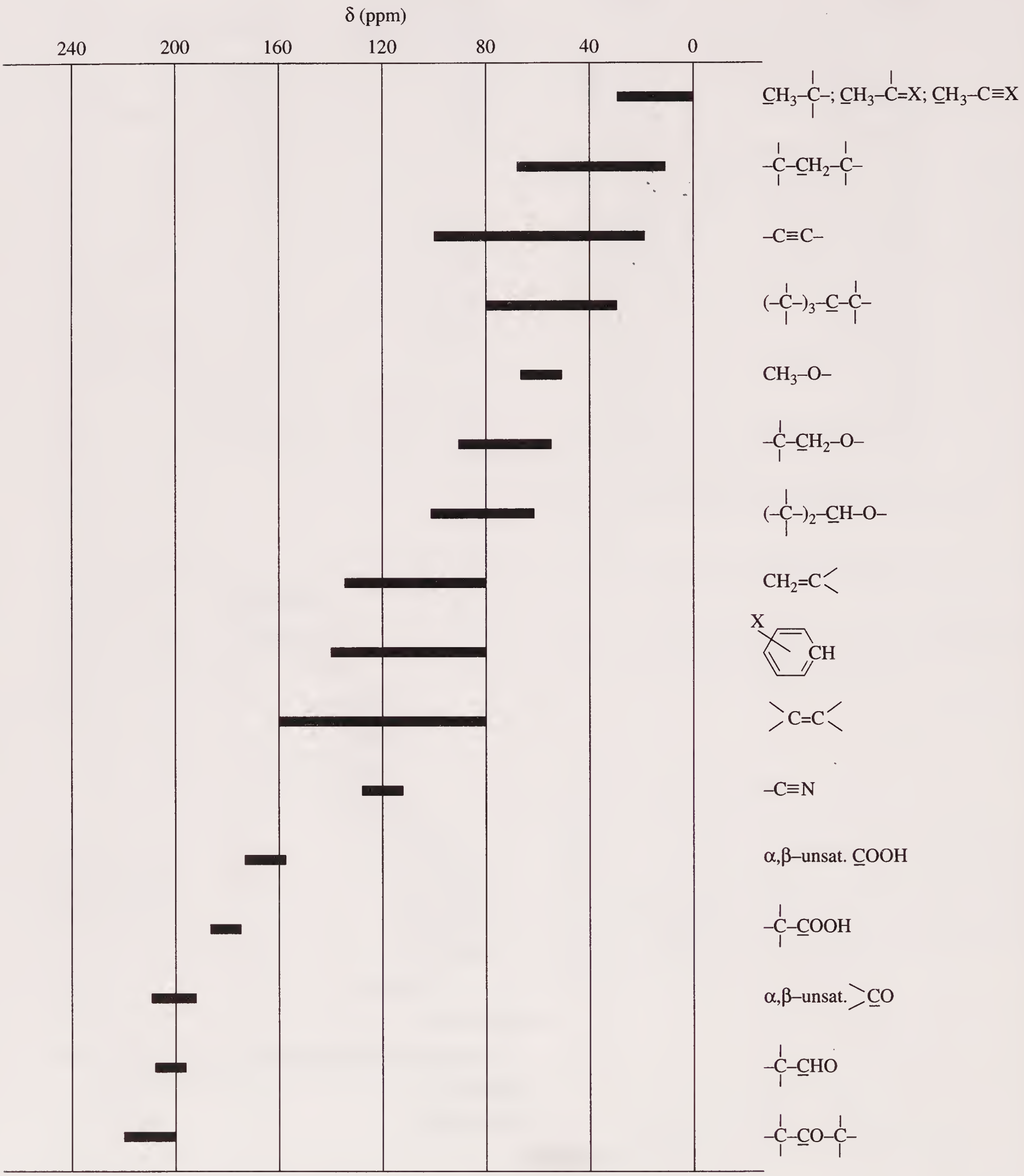


Figure 17.2 Ranges of ^{13}C nmr chemical shifts for various groups (X = any group), relative to δ(TMS) = 0.

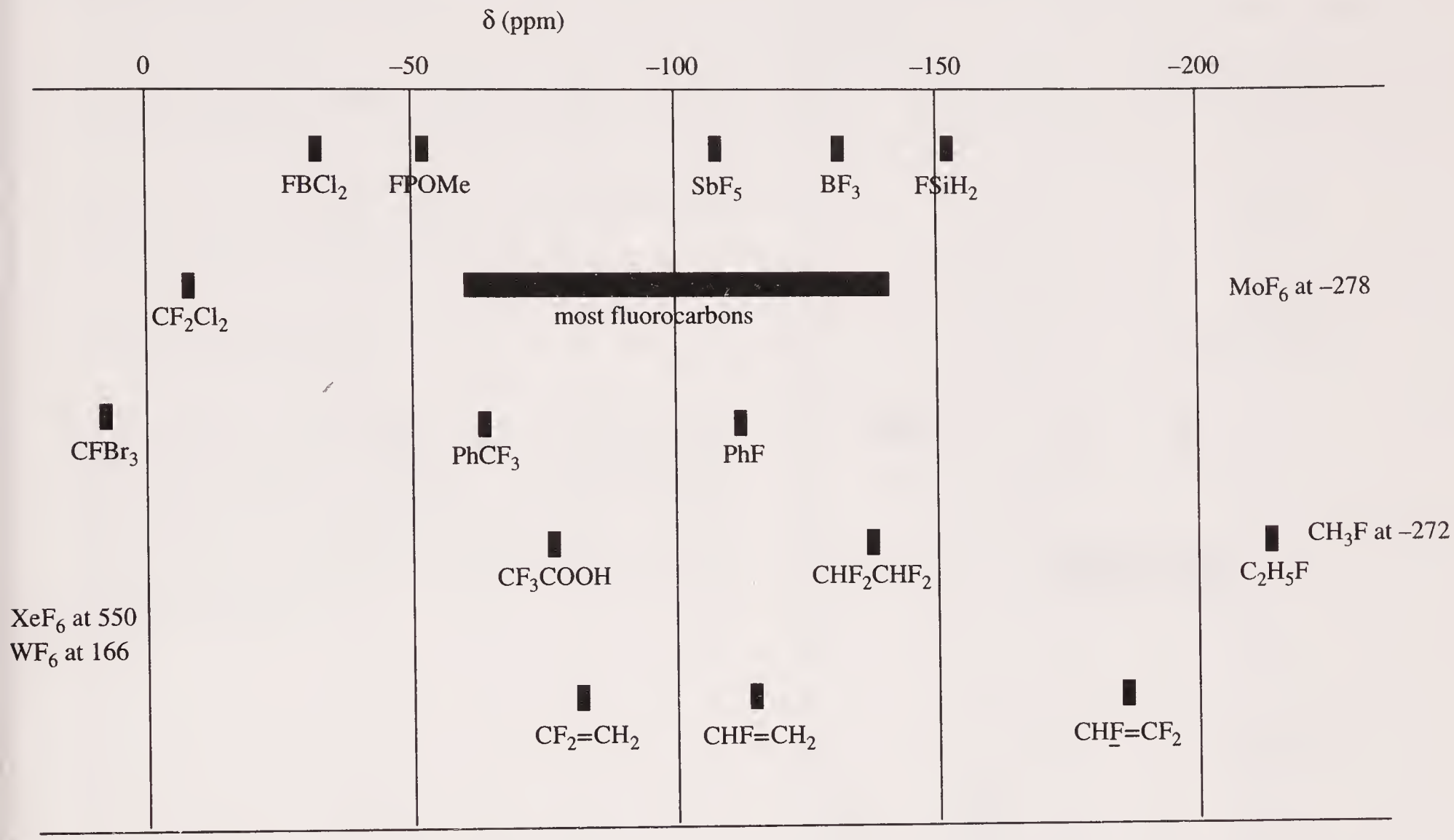


Figure 17.3 Ranges of ^{19}F nmr chemical shifts, relative to $\delta(CFCl_3) = 0$. (Reproduced with permission from W. Kemp, *NMR in Chemistry*; published by Macmillan Press Ltd, 1986).

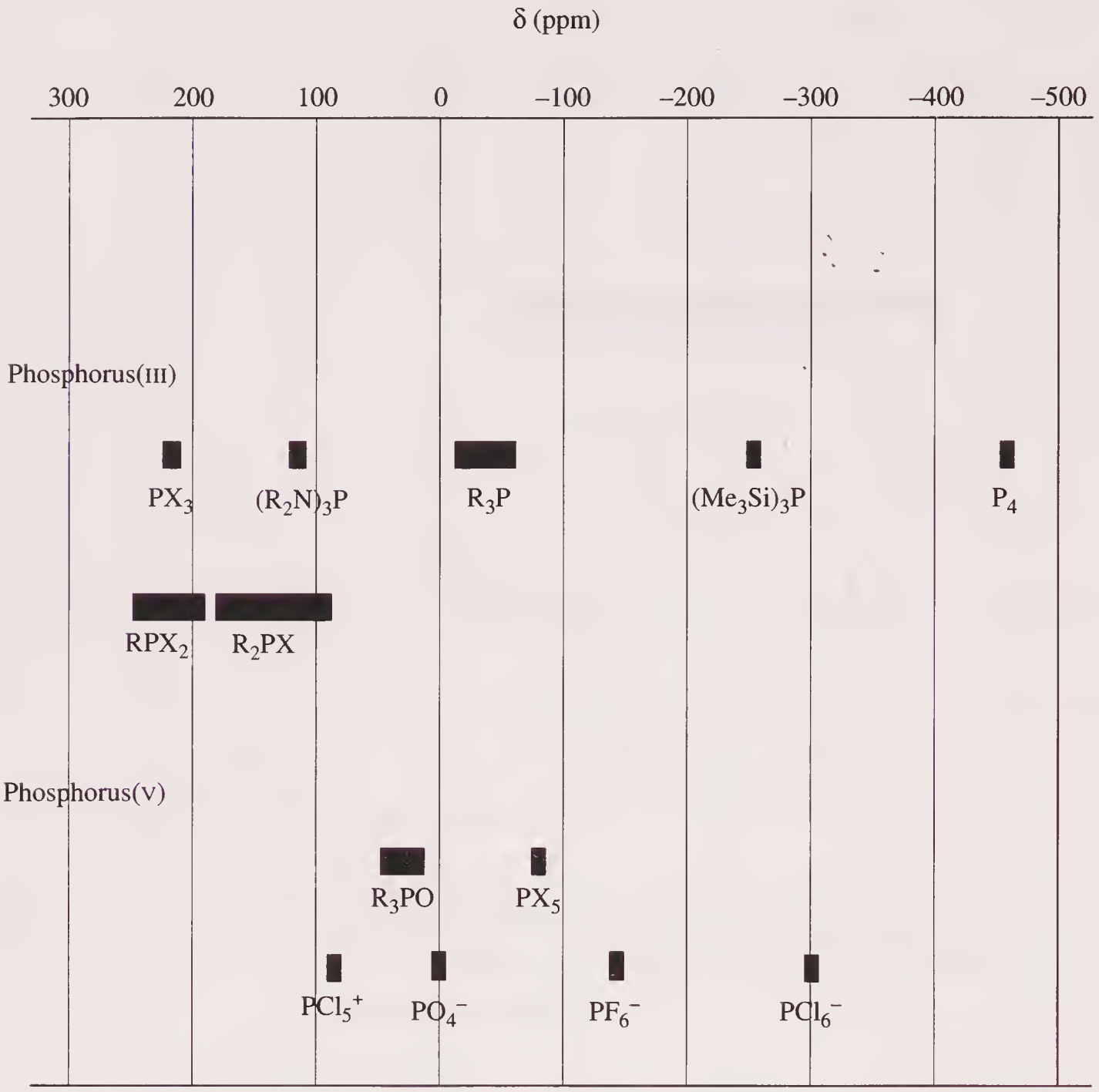


Figure 17.4 Ranges of ^{31}P nmr chemical shifts, relative to $\delta(H_3PO_4(aq)) = 0$. (Reproduced with permission from W. Kemp, *NMR in Chemistry*; published by Macmillan Press Ltd, 1986.)

17.4 Mass spectrometry

17.4.1 Natural abundance and atomic weight of isotopes

Table 17.8 lists some isotopes, along with their atomic weights and natural abundances.

17.4.2 Fragment ions

Some common fragment ions that are lost in mass spectra, and possible inferences that can be drawn from such loss, are tabulated in Table 17.9. In contrast, some common fragment ions that are found in mass spectra are listed in Table 17.10, again with possible inferences.

Table 17.8 Natural abundance and atomic weights of some isotopes

Isotope	Atomic weight (^{12}C = 12.000 000)	Natural abundance (%)
^{1}H	1.007 825	99.985
^{2}H	2.014 102	0.015
^{12}C	12.000 000	98.9
^{13}C	13.003 354	1.1
^{14}N	14.003 074	99.64
^{15}N	15.000 108	0.36
^{16}O	15.994 915	99.8
^{17}O	16.999 133	0.04
^{18}O	17.999 160	0.2
^{19}F	18.998 405	100
^{28}Si	27.976 927	92.2
^{29}Si	28.976 491	4.7
^{30}Si	29.973 761	3.1
^{31}P	30.973 763	100
^{32}S	31.972 074	95.0
^{33}S	32.971 461	0.76
^{34}S	33.967 865	4.2
^{35}Cl	34.968 855	75.8
^{37}Cl	36.965 896	24.2
^{79}Br	78.918 348	50.5
^{81}Br	80.916 344	49.5
^{127}I	126.904 352	100

Table 17.9 Some common fragments lost in mass spectra

Ions	Groups	Possible inference	Ions	Groups	Possible inference
$M-1$	H	labile H, aldehydes	$M-34$	H_2S	thiol
$M-2$	H_2		$M-35, 37$	Cl	labile chloride
$M-15$	CH_3		$M-41$	C_3H_5	propyl ester
$M-16$	O	nitro compound, sulfoxide	$M-42$	CH_2CO	methyl ketone, aryl acetate
$M-16$	NH_2	sulfonamide, carboxamide	$M-42$	C_3H_6	butyl or isobutyl ketone, aryl propyl ether
$M-17$	OH	acid, oxime	$M-43$	C_3H_7	propyl ketone, $ArCH_2CH_2CH_3$
$M-17$	NH_3		$M-43$	CH_3CO	methyl ketone
$M-18$	H_2O	alcohol, aldehyde, ketone	$M-44$	CO_2	ester, anhydride
$M-19$	F	fluoride	$M-44$	C_3H_8	
$M-20$	HF	fluoride	$M-45$	COOH	carboxylic acid
$M-26$	C_2H_2	aromatic hydrocarbon	$M-45$	OC_2H_5	ethyl ester
$M-26$	CN	aliphatic nitrile	$M-46$	C_2H_5OH	ethyl ester
$M-27$	HCN	nitrile, nitrogen heterocycle	$M-46$	NO_2	aromatic nitro compound
$M-28$	CO	quinone, phenol	$M-48$	SO	aromatic sulfoxide
$M-28$	C_2H_4	aromatic ethyl ether, propyl ketone	$M-55$	C_4H_7	butyl ester
$M-29$	CHO	alcohol	$M-56$	C_4H_8	ArR (R = butyl, 2-methyl-propyl, pentyl, 3-methyl-butyl, pentyl ketone
$M-29$	C_2H_5	ethyl ketone, $ArCH_2CH_2CH_3$, ethyl ester	$M-57$	C_4H_9	butyl ketone
$M-30$	C_2H_6		$M-57$	C_2H_5CO	ethyl ketone
$M-30$	CH_2O	aryl methyl ether	$M-58$	C_4H_{10}	
$M-30$	NO	aromatic nitro compound	$M-60$	CH_3COOH	acetate
$M-31$	OCH_3	methyl ester	$M-79, 81$	Br	bromide
$M-32$	CH_3OH	methyl ester	$M-127$	I	iodide
$M-32$	S	sulfide, aromatic thiol			
$M-33$	$H_2O + CH_3$				
$M-33$	HS	thiol			

Table 17.10 Common fragment ions in mass spectra

m/e	Ion	Possible inference
15	CH_3^+	
18	H_2O^+	
26	$C_2H_2^+$	
27	$C_2H_3^+$	
28	CO^+	carbonyl compound
28	$C_2H_4^+$	ethyl compound
28	N_2^+	azo compound
29	CHO^+	aldehyde
29	$C_2H_5^+$	ethyl compound
30	$H_2C{=}NH_2^+$	primary amine
31	$H_2C{=}OH^+$	primary alcohol
35, 37	Cl^+	chloro compound
36, 38	HCl^+	chloro compound
39	$C_3H_3^+$	
40	$C_3H_4^+$	
41	$C_3H_5^+$	
42	$C_2H_2O^+$	acetate
42	$C_3H_6^+$	
43	H_3CCO^+	H_3CCOX
43	$C_3H_7^+$	C_3H_7X
44	$C_2H_6N^+$	aliphatic amine
44	$O{=}C{=}NH_2^+$	primary amide
44	CO_2^+	
44	$C_3H_8^+$	
44	$H_2C{=}CH(OH)^+$	aldehyde
45	$H_2C{=}OCH_3^+$	ether, alcohol
45	$H_3CCH{=}OH^+$	ether, alcohol
47	$H_2C{=}SH^+$	aliphatic thiol
49, 51	H_2CCl^+	chloromethyl compound
50	$C_4H_2^+$	aromatic compound
51	$C_4H_3^+$	C_6H_5X
55	$C_4H_7^+$	unsaturated hydrocarbon
56	$C_4H_8^+$	
57	$C_4H_9^+$	C_4H_9X
57	$H_3CCH_2CO^+$	ethyl ketone, propionate ester
58	$H_2C{=}C(OH)CH_3^+$	methyl ketone, dialkyl ketone
58	$Me_2N{=}CH_2^+$	aliphatic amine
59	$COOMe^+$	methyl ester
59	$H_2C{=}C(OH)NH_2^+$	primary amide
59	$H_2C{=}OC_2H_5^+$	ether
59	$C_2H_5CH{=}OH^+$	$C_2H_5CH(OH)X$
60	$H_2C{=}C(OH)OH^+$	carboxylic acid
61	$H_3CCO(OH_2)^+$	acetate ester
61	$HSCH_2CH_2^+$	aliphatic thiol
66	$H_2S_2^+$	dialkyl disulphide
68	$N{\equiv}CCH_2CH_2CH_2^+$	RX (R = pyrrolyl)
69	CF_3^+	
69	$C_5H_9^+$	
70	$C_5H_{10}^+$	
71	$C_5H_{11}^+$	$C_5H_{11}X$
71	$C_3H_7CO^+$	propyl ketone, butyrate ester

Table continued overleaf

Table 17.10 *Continued*

m/e	Ion	Possible inference
72	$H_2C{=}C(OH)C_2H_5^+$	ethyl alkyl ketone
72	$C_3H_7CH{=}NH_2^+$	amine
73	$C_4H_9O^+$	
73	$COOEt^+$	ethyl ester
73	Me_3Si^+	Me_3SiX
74	$H_2C{=}C(OH))OCH_3^+$	methyl ester
75	$Me_2Si{=}OH^+$	Me_3SiOX
75	$C_2H_5CO(OH_2)^+$	propionate ester
76	$C_6H_4^+$	C_6H_5X, XC_6H_4Y
77	$C_6H_5^+$	C_6H_5X
78	$C_6H_6^+$	$C_6H_5^+$
78	$C_5H_4N^+$	RX (X = pyridinyl)
79	$C_6H_7^+$	C_6H_5X
79, 81	Br^+	bromo compound
80, 82	HBr^+	bromo compound
80	$C_5H_6N^+$	RCH_2X (R = pyrrolyl)
81	$C_5H_5O^+$	RCH_2X (R = pyranyl)
83, 85, 87	$HCCl_2^+$	$HCCl_3$
85	$C_6H_{13}^+$	$C_6H_{13}X$
85	$C_4H_9CO^+$	C_4H_9COX
85	$C_5H_9O^+$	RX (X = 2-pyranyl)
85	$C_4H_5O_2^+$	RX (R = 5-oxo-2-furanyl)
86	$C_4H_9CH{=}NH_2^+$	amine
86	$H_2C{=}C(OH)C_3H_7^+$	propyl alkyl ketone
87	$H_2C{=}CHC(=OH)OMe^+$	XCH_2CH_2COOMe
91	$C_7H_7^+$	$C_6H_5CH_2X$, $H_3CC_6H_4X$
91,93	$C_4H_8Cl^+$	RCl (R = n-alkyl ≥ hexyl)
92	$C_7H_8^+$	$C_6H_5CH_2R$ (R = alkyl)
92	$C_6H_6N^+$	RCH_2X (R = pyridinyl)
93, 95	$BrCH_2^+$	$BrCH_2X$
94	$C_6H_6O^+$	C_6H_5OR (R = alkyl)
94	$C_5H_4NO^+$	RCOX (R = pyrrolyl)
95	$C_5H_3O_2^+$	RCOX (R = pyranyl)
97	$C_5H_5S^+$	RCH_2X (R = thienyl)
105	$C_6H_5CO^+$	C_6H_5COX
105	$C_8H_9^+$	$H_3CC_6H_4CH_2X$
107	$C_7H_7O^+$	$HOC_6H_4CH_2X$
107, 109	$C_2H_4Br^+$	
111	$C_5H_3OS^+$	RCOX (R = thienyl)
121	$C_8H_9O^+$	$MeOC_6H_4CH_2X$
123	$C_6H_5COOH_2^+$	alkyl benzoate
127	I^+	
128	HI^+	
135, 137	$C_4H_8Br^+$	RBr (R = n-alkyl ≥ hexyl)
141	CH_2I^+	

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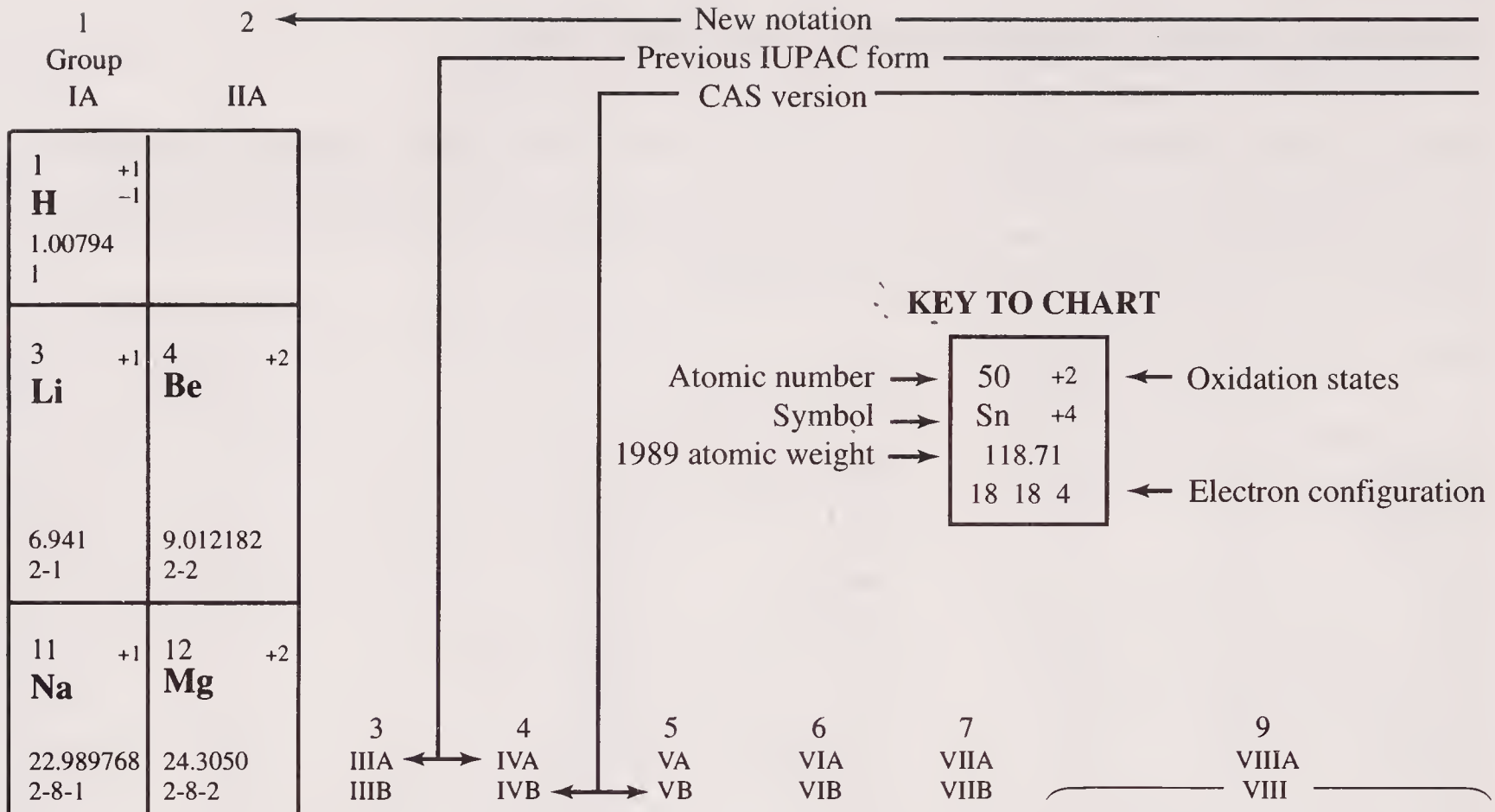
Page numbers appearing in **bold** refer to figures, and page numbers appearing in *italic* refer to tables.

Standard atomic weights of the elements (1991)

Atomic weights given are scaled to $^{12}C = 12$. The values for the atomic weights and uncertainties (in parentheses following the last significant figure to which they are attributed) apply to elements as they exist on Earth. An asterisk denotes that the element has no stable nuclides. The values in parentheses represent the atomic mass number of the radioisotope of longest known half-life.

Name	Symbol	Atomic number	Atomic weight
actinium*	Ac	89	(227)
aluminium	Al	13	26.981539(5)
americium*	Am	95	(243)
antimony	Sb	51	121.757(3)
argon	Ar	18	39.948(1)
arsenic	As	33	74.92159(2)
astatine	At	85	(210)
barium	Ba	56	137.327(7)
berkelium*	Bk	97	(247)
beryllium	Be	4	9.012182(3)
bismuth	Bi	83	208.98037(3)
boron	B	5	10.811(5)
bromine	Br	35	79.904(1)
cadmium	Cd	48	112.411(8)
caesium	Cs	55	132.90543(5)
calcium	Ca	20	40.078(4)
californium*	Cf	98	(251)
carbon	C	6	12.011(1)
cerium	Ce	58	140.115(4)
chlorine	Cl	17	35.4527(9)
chromium	Cr	24	51.9961(6)
cobalt	Co	27	58.93320(1)
copper	Cu	29	63.546(3)
curium*	Cm	96	(247)
dysprosium	Dy	66	162.50(3)
einsteinium*	Es	99	(252)
erbium	Er	68	167.26(3)
europium	Eu	63	151.965(9)
fermium*	Fm	100	(257)
fluorine	F	9	18.9984032(9)
francium*	Fr	87	(223)
gadolinium	Gd	64	157.25(3)
gallium	Ga	31	69.723(1)
germanium	Ge	32	72.61(2)
gold	Au	79	196.96654(3)
hafnium	Hf	72	178.49(2)
helium	He	2	4.002602(2)
holmium	Ho	67	164.93032(3)
hydrogen	H	1	1.00794(7)
indium	In	49	114.818(3)
iodine	I	53	126.90447(3)
iridium	Ir	77	192.22(3)
iron	Fe	26	55.847(3)
krypton	Kr	36	83.80(1)
lanthanum	La	57	138.9055(2)
lawrencium*	Lr	103	(262)
lead	Pb	82	207.2(1)
lithium	Li	3	6.941(2)
lutetium	Lu	71	174.967(1)
magnesium	Mg	12	24.3050(6)
manganese	Mn	25	54.93805(1)
mendelevium*	Md	101	(258)
mercury	Hg	80	200.59(2)
molybdenum	Mo	42	95.94(1)
neodymium	Nd	60	144.24(3)
neon	Ne	10	20.1797(6)
neptunium*	Np	93	(237)
nickel	Ni	28	58.6934(2)
niobium	Nb	41	92.90638(2)
nitrogen	N	7	14.00674(7)
nobelium*	No	102	(259)
osmium	Os	76	190.23(3)
oxygen	O	8	15.9994(3)
palladium	Pd	46	106.42(1)
phosphorus	P	15	30.973762(4)
platinum	Pt	78	195.08(3)
plutonium*	Pu	94	(244)
polonium*	Po	84	(209)
potassium	K	19	39.0983(1)
praseodymium	Pr	59	140.90765(3)
promethium*	Pm	61	(145)
protactinium*	Pa	91	231.03588(2)
radium*	Ra	88	(226)
radon*	Rn	86	(222)
rhenium	Re	75	186.207(1)
rhodium	Rh	45	102.90550(3)
rubidium	Rb	37	85.4678(3)
ruthenium	Ru	44	101.07(2)
samarium	Sm	62	150.36(3)
scandium	Sc	21	44.955910(9)
selenium	Se	34	78.96(3)
silicon	Si	14	28.0855(3)
silver	Ag	47	107.8682(2)
sodium	Na	11	22.989768(6)
strontium	Sr	38	87.62(1)
sulfur	S	16	32.066(6)
tantalum	Ta	73	180.9479(1)
technetium*	Tc	43	(98)
tellurium	Te	52	127.60(3)
terbium	Tb	65	158.92534(3)
thallium	Tl	81	204.3833(2)
thorium	Th	90	232.0381(1)
thulium*	Tm	69	168.93421(3)
tin	Sn	50	118.710(7)
titanium	Ti	22	47.88(3)
tungsten	W	74	183.84(1)
unnilhexium*	Unh	106	(263)
unnilpentium*	Unp	105	(262)
unnilquadium*	Unq	104	(261)
unnilseptium*	Uns	107	(262)
uranium*	U	92	238.0289(1)
vanadium	V	23	50.9415(1)
xenon	Xe	54	131.29(2)
ytterbium	Yb	70	173.04(3)
yttrium	Y	39	88.90585(2)
zinc	Zn	30	65.39(2)
zirconium	Zr	40	91.224(2)

For full details, see *Pure Appl. Chem.*, 1992, **64**, 1520.



1 Group IA	2 IIA	3 IIIA IIIB	4 IVA IVB	5 VA VB	6 VIA VIB	7 VIIA VIIB	9 VIIIA VIII		
1 +1 −1 **H** 1.00794 1									
3 +1 **Li** 6.941 2-1	4 +2 **Be** 9.012182 2-2								
11 +1 **Na** 22.989768 2-8-1	12 +2 **Mg** 24.3050 2-8-2								
19 +1 **K** 39.0983 -8-8-1	20 +2 **Ca** 40.078 -8-8-2	21 +3 **Sc** 44.955910 -8-9-2	22 +2 +3 +4 **Ti** 47.867 -8-10-2	23 +2 +3 +4 +5 **V** 50.9415 -8-11-2	24 +2 +3 +6 **Cr** 51.9961 -8-13-1	25 +2 +3 +4 +7 **Mn** 54.93085 -8-13-2	26 +2 +3 **Fe** 55.845 -8-14-2	27 +2 +3 **Co** 58.93320 -8-15-2	28 +2 +3 **Ni** 58.6934 -8-16-2
37 +1 **Rb** 85.4678 -18-8-1	38 +2 **Sr** 87.62 -18-8-2	39 +3 **Y** 88.90585 -18-9-2	40 +4 **Zr** 91.224 -18-10-2	41 +3 +5 **Nb** 92.90638 -18-12-1	42 +6 **Mo** 95.94 -18-13-1	43 +4 +6 +7 **Tc** (98) -18-13-2	44 +3 **Ru** 101.07 -18-15-1	45 +3 **Rh** 102.90550 -18-16-1	46 +2 +4 **Pd** 106.42 -18-18-0
55 +1 **Cs** 132.90543 -18-8-1	56 +2 **Ba** 137.327 -18-8-2	57* +3 **La** 138.9055 -18-9-2	72 +4 **Hf** 178.49 -32-10-2	73 +5 **Ta** 180.9479 -32-11-2	74 +6 **W** 183.84 -32-12-2	75 +4 +6 +7 **Re** 186.207 -32-13-2	76 +3 +4 **Os** 190.23 -32-14-2	77 +3 +4 **Ir** 192.217 -32-15-2	78 +2 +4 **Pt** 195.08 -32-16-2
87 +1 **Fr** (223) -18-8-1	88 +2 **Ra** 226.025 -18-8-2	89** +3 **Ac** 227.028 -18-9-2	104 +4 **Db** (261) -32-10-2	105 **Jl** (262) -32-11-2	106 **Rf** (263) -32-12-2	107 **Bh** (262) -32-13-2			

*Lanthanides	58 +3 +4 **Ce** 140.115 -19-9-2	59 +3 **Pr** 140.90765 -21-8-2	60 +3 **Nd** 144.24 -22-8-2	61 +3 **Pm** (145) -23-8-2	62 +3 +3 **Sm** 150.36 -24-8-2	63 +2 +3 **Eu** 151.965 -25-8-2	64 +3 **Gd** 157.25 -25-9-2	65 +3 **Tb** 158.92534 -27-8-2	
**Actinides	90 +4 **Th** 232.0381 -18-10-2	91 +5 +4 **Pa** 231.03588 -20-9-2	92 +3 +4 +5 +6 **U** 238.0289 -21-9-2	93 +3 +4 +5 +6 **Np** 237.048 -22-9-2	94 +3 +4 +5 +6 **Pu** (244) -24-8-2	95 +3 +4 +5 +6 **Am** (243) -25-8-2	96 +3 **Cm** (247) -25-9-2	97 +3 +4 **Bk** (247) -27-8-2	

The new IUPAC format numbers the groups from 1 to 18. The previous IUPAC numbering system and the system used by Chemical Abstracts Service (CAS) are also shown. For radioactive elements that do not occur in Nature, the mass number of the most stable isotope is given in parentheses.

of the elements

		13 IIIB IIIA	14 IVB IVA	15 VB VA	16 VIB VIA	17 VIIB VIIA	18 VIIIA	Shell
							2 0 **He** 4.0020602 2	K
		5 +3 **B** 10.811 2-3	6 +2 +4 −4 **C** 12.011 2-4	7 +1 +2 +3 +4 +5 −1 −2 −3 N 14.00674 2-5	8 −2 **O** 15.9994 2-6	9 −1 **F** 18.9984032 2-7	10 0 **Ne** 20.1797 2-8	K-L
		13 +3 **Al** 26.981539 2-8-3	14 +2 +4 −4 **Si** 28.0855 2-8-4	15 +3 +5 −3 **P** 30.97362 2-8-5	16 +4 +6 −2 **S** 32.066 2-8-6	17 +1 +5 +7 −1 **Cl** 35.4527 2-8-7	18 0 **Ar** 39.948 2-8-8	K-L-M
11 IB	12 IIB							
29 +1 +2 **Cu** 63.546 -8-18-1	30 +2 **Zn** 65.39 -8-18-2	31 +3 **Ga** 69.723 -8-18-3	32 +2 +4 **Ge** 72.61 -8-18-4	33 +3 +5 −3 **As** 74.92159 -8-18-5	34 +4 +6 −2 **Se** 78.96 -8-18-6	35 +1 +5 −1 **Br** 79.904 -8-18-7	36 0 **Kr** 83.80 -8-18-8	-L-M-N
47 +1 **Ag** 107.8682 -18-18-1	48 +2 **Cd** 112.411 -18-18-2	49 +3 **In** 114.818 -18-18-3	50 +2 +4 **Sn** 118.710 -18-18-4	51 +3 +5 −3 **Sb** 121.760 -18-18-5	52 +4 +6 −2 **Te** 127.60 -18-18-6	53 +1 +5 +7 −1 **I** 126.90447 -18-18-7	54 0 **Xe** 131.29 -18-18-8	-M-N-O
79 +1 +3 **Au** 196.96654 -32-18-1	80 +1 +2 **Hg** 200.59 -32-18-2	81 +1 +3 **Tl** 204.3833 -32-18-3	82 +2 +4 **Pb** 207.2 -32-18-4	83 +3 +5 **Bi** 208.98037 -32-18-5	84 +2 +4 **Po** (209) -32-18-6	85 **At** (210) -32-18-7	86 0 **Rn** (222) -32-18-8	-N-O-P
								-O-P-Q

66 +3 **Dy** 162.50 -28-8-2	67 +3 **Ho** 164.93032 -29-8-2	68 +3 **Er** 167.26 -30-8-2	69 +3 **Tm** 168.93421 -31-8-2	70 +2 +3 **Yb** 173.04 -32-8-2	71 +3 **Lu** 174.967 -32-9-2	-N-O-P
98 +3 **Cf** (251) -28-8-2	99 +3 **Es** (252) -29-8-2	100 +3 **Fm** (257) -30-8-2	101 +2 +3 **Md** (258) -31-8-2	102 +2 +3 **No** (259) -32-8-2	103 +3 **Lr** (260) -32-9-2	-O-P-Q

From *CRC Handbook of Chemistry and Physics*, 75th edn, 1994–1995

Multiples of element weights

C	12.01	H_5	5.040	H_{60}	60.48	$(OCH_3)_7$	217.24
C_2	24.02	H_6	6.048	H_{61}	61.49	$(OCH_3)_8$	248.27
C_3	36.03	H_7	7.056	H_{62}	62.50		
C_4	48.04	H_8	8.064	H_{63}	63.50	OC_2H_5	45.06
C_5	60.05	H_9	9.072	H_{64}	64.51	$(OC_2H_5)_2$	90.12
C_6	72.06	H_{10}	10.08	H_{65}	65.52	$(OC_2H_5)_3$	135.18
C_7	84.07	H_{11}	11.09			$(OC_2H_5)_4$	180.24
C_8	96.08	H_{12}	12.10	O	16	$(OC_2H_5)_5$	225.30
C_9	108.09	H_{13}	13.10	O_2	32		
C_{10}	120.10	H_{14}	14.11	O_3	48	$OCOCH_3$	59.04
C_{11}	132.11	H_{15}	15.12	O_4	64	$(OCOCH_3)_2$	118.09
C_{12}	144.12	H_{16}	16.13	O_5	80	$(OCOCH_3)_3$	177.13
C_{13}	156.13	H_{17}	17.14	O_6	96	$(OCOCH_3)_4$	236.18
C_{14}	168.14	H_{18}	18.14	O_7	112	$(OCOCH_3)_5$	295.22
C_{15}	180.15	H_{19}	19.15	O_8	128	$(OCOCH_3)_6$	354.26
C_{16}	192.16	H_{20}	20.16	O_9	144	$(OCOCH_3)_7$	413.31
C_{17}	204.17	H_{21}	21.17	O_{10}	160	$(OCOCH_3)_8$	472.35
C_{18}	216.18	H_{22}	22.18			$(OCOCH_3)_9$	531.40
C_{19}	228.19	H_{23}	23.18	N	14.007	$(OCOCH_3)_{10}$	590.44
C_{20}	240.20	H_{24}	24.19	N_2	28.02		
C_{21}	252.21	H_{25}	25.20	N_3	42.02	$(H_2O)_{0.5}$	9.01
C_{22}	264.22	H_{26}	26.21	N_4	56.03	H_2O	18.02
C_{23}	276.23	H_{27}	27.22	N_5	70.04		
C_{24}	288.24	H_{28}	28.22	N_6	84.05	$(H_2O)_{1.5}$	27.02
C_{25}	300.25	H_{29}	29.23			$(H_2O)_2$	36.03
C_{26}	312.26	H_{30}	30.24	S	32.064	$(H_2O)_3$	54.05
C_{27}	324.27	H_{31}	31.25	S_2	61.12	$(H_2O)_4$	72.06
C_{28}	336.28	H_{32}	32.26	S_3	96.19	$(H_2O)_5$	90.08
C_{29}	348.29	H_{33}	33.26	S_4	128.26	$(H_2O)_6$	108.10
C_{30}	360.30	H_{34}	34.27				
C_{31}	372.31	H_{35}	35.28	F	19.00	P	30.974
C_{32}	384.32	H_{36}	36.29	F_2	38.00	P_2	61.948
C_{33}	396.33	H_{37}	37.30	F_3	57.00	P_3	92.922
C_{34}	408.34	H_{38}	38.30			P_4	123.90
C_{35}	420.35	H_{39}	39.31	Cl	35.453		
C_{36}	432.36	H_{40}	40.32	Cl_2	70.91	Na	22.990
C_{37}	444.37	H_{41}	41.33	Cl_3	106.37	Na_2	45.98
C_{38}	456.38	H_{42}	42.34	Cl_4	141.83	Na_3	68.97
C_{39}	468.39	H_{43}	43.34	Cl_5	177.28		
C_{40}	480.40	H_{44}	44.35			K	39.10
C_{41}	492.41	H_{45}	45.36	Br	79.909	K_2	78.20
C_{42}	504.42	H_{46}	46.37	Br_2	159.82	K_3	117.30
C_{43}	516.43	H_{47}	47.38	Br_3	239.73		
C_{44}	528.44	H_{48}	48.38	Br_4	319.64	Ag	107.87
C_{45}	540.45	H_{49}	49.39			Ag_2	215.74
C_{46}	552.46	H_{50}	50.40	I	126.90		
C_{47}	564.47	H_{51}	51.41	I_2	253.80	Cu	63.54
C_{48}	576.48	H_{52}	52.42	I_3	380.70	Cu_2	127.08
C_{49}	588.49	H_{53}	53.42			Cr	52.00
C_{50}	600.50	H_{54}	54.43	OCH_3	31.03	Hg	200.59
		H_{55}	55.44	$(OCH_3)_2$	62.07	Pb	207.19
H	1.008	H_{56}	56.45	$(OCH_3)_3$	93.10	Pt	195.09
H_2	2.016	H_{57}	57.46	$(OCH_3)_4$	124.14	Se	78.96
H_3	3.024	H_{58}	58.46	$(OCH_3)_5$	155.17		
H_4	4.032	H_{59}	59.47	$(OCH_3)_6$	186.20		

From *The Aldrich Catalogue*

The Organic Chemist's Desk Reference

A COMPANION VOLUME TO THE
DICTIONARY OF ORGANIC COMPOUNDS, SIXTH EDITION

P.H. Rhodes
With contributions from other DOC editors and contributors

The Organic Chemist's Desk Reference is packed with invaluable information and is a handy guide to the techniques and methods of organic chemistry.

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The cover illustration is a polarised light micrograph of crystals of D-Sorbitol. *Sidney Moulds/Science Photo Library.*

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