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ORGANIC CHEMISTRY DIVISION
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY (III.1)
COMMISSION ON PHYSICAL ORGANIC CHEMISTRY (III.2)

# GLOSSARY OF CLASS NAMES OF ORGANIC COMPOUNDS AND REACTIVE INTERMEDIATES BASED ON STRUCTURE

(IUPAC Recommendations 1995)

### Prepared for publication by

#### G.P. MOSS, P.A.S. SMITH and D. TAVERNIER

Composition of the III.1 & III.2 Working Party (1980-1994): H.J.T. Bos, A.J. Boulton, E.W. Godly, P. Grünanger, A.D. McNaught, G.P. Moss, R. Panico, J. Rigaudy, P.A.S. Smith (Convenor from III.1), J.H. Stocker, D. Tavernier, R.A.Y. Jones, J. March, J.M. McBride, P. Müller (Convenor from III.2).

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# Glossary of class names of organic compounds and reactive intermediates based on structure (IUPAC Recommendations 1995)

Synopsis. This is a glossary of terms used to denote classes of compounds, substituent groups and reactive intermediates, in contrast to individual compounds. The overwhelming majority of the terms refer to organic compounds, but a few classes that may be considered inorganic are included for convenience. The principal criterion for inclusion is that the class be definable by structure.

### Introduction

A class is a set of compounds sharing a common structural feature to which is attached a variable part (or parts) defining a specific compound of the class. The common feature is often a functional group to which one or a small number of variable parts are attached (e.g. aldehydes, ketones). The variable parts are in this glossary represented by hydrocarbyl groups (q.v.). The most simple representation of a class is thus defined. However membership of one class need not exclude membership of another class, and certain substitutions, as e.g. with heterocyclyl groups (q.v.) linked through a carbon atom in the R group, may be allowed. For instance, ethylamine as well as [1-(furan-2-yl)ethyl]amine and (2-methoxyethyl)amine belong to the class amines. The common feature may also be a sizeable part of the molecular structure, or a repetitive part of the molecular structure, possibly but not necessarily devoid of functionalities (e.g. steroids, terpenoids); quite often the attached variable groups may be many and of any functionality.

Classes defined by use, characteristics, or origin are excluded. Class names that are plurals of systematic names for parent compounds are occasionally cited. Some terms are included that are not actually class names, but are commonly encountered components of class names. These are mostly prefixes, and defining their meanings permits a host of class names beginning with them to be dispensed with.

There is some overlap with other IUPAC documents, especially the 'Glossary of Terms Used in Physical-Organic Chemistry'. Because the viewpoints are sometimes different, the wording of the definitions may in a few cases differ but most are reproduced verbatim.

The recommended class names, which are signalled by an asterisk, respect IUPAC nomenclature as presented in the 'Blue Book' (Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H, 1979 edition), the 'Revised Nomenclature for Radicals, Ions, Radical Ions and Related Species, Recommendations 1992' and A Guide to IUPAC Nomenclature of Organic Chemistry, Recommendations 1993, (including Revisions, Published and hitherto Unpublished, to the 1979 Edition of Nomenclature of Organic Chemistry).

Some class names are explicitly defined in the Blue Book, for others the meaning is implicit. Many more class names are to be found in the chemical literature. A selection of the more important ones appears in this glossary. Some class names occurring mainly in the older literature have been included too. The compilers have considered customary usage and the need for clearly defined limits of meaning. Some compromises were necessary, but the definitions have survived scrutiny by the Commissions and consultants.

Recommended class names carry a reference to an official IUPAC publication. The status of the remaining entries varies from unreserved acceptance to outright rejection. Class names not derived from an official source may carry a reference to other literature (a preference for the cited text over others is not implied). The definition of rejected class names is for information only; reasons for rejection are usually cited or indicated, and a cross-reference to the preferred class name is given.

A compound may belong to two or more different classes, e.g. it may be a ketone as well as an ester. Quite often composite names are then used, one class being denoted by an adjective, the second by a noun. The adjective and noun are separated by a space, thus oxo ester. However in the name of a specific compound there is no space between the prefix, indicating a specific substituent, and the name of the parent. Contrast e.g.  $\alpha$ -amino carboxylic acids (class name) and 2-aminopentanoic acid (specific compound name).

# **Symbols**

An asterisk (\*) on an entry indicates that the definition is based on the contents of an official IUPAC source. Italicisation marks a relevant entry used in the definition of another entry. In formulae, charges are not circled and non-bonding electrons are not shown. However, in carbenes and related molecules, one electron pair is shown as a reminder of their lower-than-standard valency state. The dipolar bonds in sulfoxides, sulfones, etc., are represented by formal double bonds. In the formulae to be found in the definitions, the symbol R means any hydrocarbyl group (q.v.) or H, unless its meaning is specifically qualified. When more than one R appears, it is to be understood that the R's may be the same or different, unless otherwise indicated. Two or more R's may be linked so as to form a ring, without changing the definition  $(e.g. R_2C=0)$  includes cyclopentanone as well as pentan-3-one and pentan-2-one). M indicates a metal or metal ion, Ar means an aryl group and Ph a phenyl group.

The abbreviations used for some frequently cited sources are as follows:

BNRD: Biochemical Nomenclature and Related Documents, Portland Press, London, 1992.

2-Carb: Nomenclature of Carbohydrates, revised 1994, in preparation.

CBN: Commission on Biochemical Nomenclature. IUPAC-IUB

CNIC: Commission on Nomenclature of Inorganic Chemistry, IUPAC.

CNOC: Commission on Nomenclature of Organic Chemistry, IUPAC.

CPOC: Commission on Physical Organic Chemistry, IUPAC.

EJB: European Journal of Biochemistry.

GNOC: A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993, (including Revisions, Published and hitherto Unpublished, to the 1979 Edition of Nomenclature of Organic Chemistry), Blackwell Scientific Publications, Oxford, 1993.

GTPOC: Glossary of Terms Used in Physical Organic Chemistry, PAC 66, 1077-1184 (1994).

JCBN: Joint Commission on Biochemical Nomenclature, IUBMB-IUPAC.

NOC: Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, Pergamon Press, Oxford, 1979.

PAC: Pure and Applied Chemistry.

RNRI: Revised Nomenclature for Radicals, Ions, Radical Ions and Related Species, Recommendations 1993, PAC 65, 1357-1455 (1993).

# Glossary

#### acenes:\*

Polycyclic aromatic *hydrocarbons* consisting of fused benzene rings in a rectilinear arrangement. NOC Rule A-21.2, GNOC Recom. R-2.4.1.3.1.

$$n = 1, 2, 3..$$

## acetals:\*

Compounds having the structure  $R_2C(OR')_2$  ( $R' \neq H$ ) and thus diethers of geminal *diols*. Originally, the term was confined to derivatives of *aldehydes* (one R = H), but now it applies equally to derivatives of *ketones* (neither R = H). NOC Rule C-331, GNOC Recom. R-5.6.4.1. Mixed acetals have different R' groups. See also *acetonides*, *ketals*. Cf. acylals, hemiacetals.

#### aldoketoses:\*

A now less preferred synonym for ketoaldoses. 2-Carb-1.5.

#### aldonic acids: \*

Polyhydroxy acids having the general formula  $HOCH_2[CH(OH)]_nC(=O)OH$  and therefore derived from an aldose by oxidation of the aldehyde function. 2-Carb-1.9. E.g.  $O_{OC}OH$ 

#### aldoses:\*

Aldehydic parent sugars (polyhydroxyaldehydes  $H[CH(OH)]_nC(=O)H$ ,  $n \ge 2$ ) and their intramolecular hemiacetals. 2-Carb-1.2. See also monosaccharides. E.g. D-glucose

#### aldoximes:\*

Oximes of aldehydes: RCH=NOH. GNOC Recom. R-5.6.6.1.

#### alicyclic compounds:

Aliphatic compounds having a carbocyclic ring structure which may be saturated or unsaturated, but may not be a benzenoid or other aromatic system.

# aliphatic compounds:

Acyclic or cyclic, saturated or unsaturated carbon compounds, excluding aromatic compounds.

# alkaloids:

Basic nitrogen compounds (mostly heterocyclic) occurring mostly in the plant kingdom (but not excluding those of animal origin). Amino acids, peptides, proteins, nucleotides, nucleic acids, amino sugars, and antibiotics are not normally regarded as alkaloids. By extension, certain neutral compounds biogenetically related to basic alkaloids are included.

#### alkanes:\*

Acyclic branched or unbranched *hydrocarbons* having the general formula  $C_nH_{2n+2}$ , and therefore consisting entirely of hydrogen atoms and saturated carbon atoms. NOC Rule A-1.1. *Cf. cycloalkanes*.

## alkanium ions:

Carbocations derived from alkanes by C-hydronation containing at least one pentacoordinate carbon atom. RNRI Rule RC-82.1.1.2. Cf. carbonium ions. E.g.  ${}^+$ CH<sub>5</sub> methanium,  $[C_2H_7]^+$  ethanium.

# alkenes:\*

Acyclic branched or unbranched hydrocarbons having one carbon-carbon double bond and the general formula  $C_nH_{2n}$ . Acyclic branched or unbranched hydrocarbons having more than one double bond are alkadienes, alkatrienes, etc. NOC Rule A-3.1. See also olefins.

2. Salts formed by replacement of a nitrogen-bound hydron of aniline by a metal or other cation. E.g. NaNHPh sodium anilide.

#### annulenes:\*

Mancude monocyclic hydrocarbons without side chains of the general formula  $C_nH_n$  (n is an even number) or  $C_nH_{n+1}$  (n is an odd number). In systematic nomenclature an annulene with seven or more carbon atoms may be named [n]annulene, where n is the number of carbon atoms. GNOC Recom. R-2.3.1.2. E.g. [9]annulene for cyclonona-1,3,5,7-tetraene.

# annulenylidenes:

Carbenes, derived by formal insertion of a divalent carbon atom into an even-membered annulene.

E.g.



cycloheptatrienylidene

### ansa compounds:

Benzene derivatives having para positions (or meta) bridged by a chain (commonly 10 to 12 atoms long) (Latin ansa, handle). By extension, any arene bridged by a chain constrained to lie over one of the two faces of the arene. Cf. cyclophanes.



# anthocyanidins:

Aglycons of anthocyanins; they are oxygenated derivatives of flavylium (2-phenylchromenylium) salts. Cf. flavonoids.

# anthocyanins:

Plant pigments of the *flavonoid* class; they are *glycosides* that on hydrolysis yield coloured *aglycons* called *anthocyanidins*.

#### antiaromatic compounds:

Compounds that contain 4n  $(n \neq 0)$   $\pi$ -electrons in a cyclic planar, or nearly planar, system of alternating single and double bonds. Cf. aromatic compounds. E.g. cyclobuta-1,3-diene.

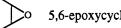
#### arenes:\*

Monocyclic and polycyclic aromatic hydrocarbons. NOC Rule A-12.4. See aromatic compounds.

# arene epoxides:

Epoxides derived from arenes by 1,2-addition of an oxygen atom to a formal double bond.

E.g.



5,6-epoxycyclohexa-1,3-diene.

(Common usage has extended the term to include examples with the epoxy group bridging nonadjacent atoms.)

arene oxides: See arene epoxides.

#### arenium ions:

Cations derived formally by the addition of a hydron or other cationic species to any position of an arene.  $E.g. C_6H_7^+$ , benzenium. Cf. aryl cations.

#### arsinic acids:\*

H<sub>2</sub>As(=0)OH and its As-hydrocarbyl derivatives. NOC Rule D-5.51. E.g. Me<sub>2</sub>As(=0)OH dimethylarsinic acid.

arsinidenes: See arsanylidenes.

#### arsinous acids:\*

H<sub>2</sub>AsOH and its As-hydrocarbyl derivatives. NOC Rule D-5.21.

### arsonic acids:\*

HAs(=O)(OH)<sub>2</sub> and its As-hydrocarbyl derivatives. NOC Rule D-5.51.

# arsonium compounds:\*

Salts (including hydroxides)  $[R_4As]^+X^-$  containing tetracoordinate arsonium ion and the associated anion. NOC Rule D-5.31. See also *onium compounds*.

#### arsonous acids:\*

HAs(OH)<sub>2</sub> and its As-hydrocarbyl derivatives. NOC Rule D-5.21.

o-tolyl.

#### arsoranes:\*

The mononuclear hydride AsH<sub>5</sub>, systematically named  $\lambda^5$ -arsane, and its hydrocarbyl derivatives. NOC Rule D-5.71. See also arsanes. By extension the term also applies to arsonium ylides. See under ylides.

# aryl cations:

Carbocations formally derived by removal of a hydride ion from a ring carbon atom of an arene. Cf. arenium ions. E.g.,

# aryl groups:\*

Groups derived from *arenes* by removal of a hydrogen atom from a ring carbon atom. NOC Rule A-13.5. Groups similarly derived from *heteroarenes* are sometimes subsumed in this definition (see *heteroaryl groups*). E.g. CH<sub>3</sub>

#### arylene groups:\*

Bivalent groups derived from *arenes* by removal of a hydrogen atom from two ring carbon atoms. A synonym is arenediyl groups. NOC Rule A-13.5. E.g.

#### arynes:

Hydrocarbons derived formally from arenes by the abstraction of two hydrogen atoms from adjacent carbon atoms; thus 1,2-didehydroarenes. Arynes are commonly represented with a formal triple bond. Cf. benzynes, dehydroarenes, heteroarynes. E.g. benzyne

azamines: See isodiazenes.

# azanes:

Saturated acyclic nitrogen hydrides having the general formula  $N_nH_{n+2}$ .

#### azides:\*

1. Compounds bearing the group  $-N_3$ , viz.  $-N=N^+=N^-$ ; usually attached to carbon. NOC Rule C-941.1. E.g. PhN<sub>3</sub> phenyl azide or azidobenzene. 1330

# cyclitols:\*

Hydroxylated *cycloalkanes* containing at least three hydroxy groups, each attached to a different ring carbon atom. BNRD, Nomenclature of Cyclitols (p. 149).

# cycloalkanes:\*

Saturated monocyclic hydrocarbons (with or without side chains). See alicyclic compounds. NOC Rule A-11.1. E.g.  $H_2C - CH_2$  cyclobutane. Unsaturated monocyclic hydrocarbons having one endocyclic double  $H_2C - CH_2$ 

or one triple bond are called cycloalkenes and cycloalkynes, respectively. Those having more than one such multiple bond are cycloalkadienes, cycloalkatrienes, etc. The inclusive terms for any cyclic hydrocarbons having any number of such multiple bonds are cyclic olefins or cyclic acetylenes.

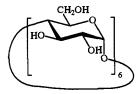
# cycloalkyl groups:\*

Univalent groups derived from cycloalkanes by removal of a hydrogen atom from a ring carbon atom. E.g. CH<sub>3</sub>-HC\_CH- 2-methylcyclopropyl. NOC Rules A-11.1, A-11.2.

cyclodepsipeptides: See depsipeptides.

# cyclodextrins:

Cyclic oligoglucosides containing 5 to ca. 10 glucose residues in which an enclosed tubular space allows reception of a guest molecule to form a *clathrate*. The synonymous term Schardinger dextrins is not recommended. ( $\alpha$ -Cyclodextrin has 6 glucose residues;  $\beta$ -cyclodextrin has 7.) Semi-systematically  $\alpha$ -cyclodextrin is called cyclomaltohexaose. 2-Carb-37.4.1. See also *dextrins*.



#### cyclohexadienyl cations:

A subclass of arenium ions.

#### cyclophanes:

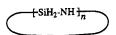
The term originally applied to compounds having two p-phenylene groups held face to face by  $-[CH_2]_n$ -bridges. It now designates compounds having (i) mancude-ring systems, or assemblies of mancude-ring systems, and (ii) atoms and/or saturated or unsaturated chains as alternate components of a large ring. GNOC Recom. R-2.4.5. Many chemists include in this class any bridged aromatic system, irrespective of the attachment positions of the bridge. E.g. [2.2](1,4)(1,4)cyclophane or

[2.2](1,4)(1,4)cyclophane or 1(1,4),4(1,4)-dibenzenacyclophane according to the provisional CNOC document on Phane Nomenclature, Part 1.

F.N. Diederich, Cyclophanes, The Royal Society of Chemistry, 1991.

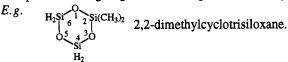
#### cyclosilazanes:\*

Compounds having rings of alternating silicon and nitrogen atoms: NOC Rule D-6.42.



# cyclosiloxanes:\*

Compounds having rings of alternating silicon and oxygen atoms. NOC Rule D-6.23.



hetarenes: Synonymous with heteroarenes.

hetaryl groups: Synonymous with heteroaryl groups.

hetarynes: Synonymous with heteroarynes.

#### heteroalkenes:

Analogues of alkenes in which a doubly bonded carbon atom is replaced by a heteroatom. E.g.  $H_2Si=CH_2$  methylidenesilane (silene less preferred),  $MeN=CH_2$  N-methylmethanimine.

#### heteroarenes:

Heterocyclic compounds formally derived from *arenes* by replacement of one or more methine (-C=) and/or vinylene (-CH=CH-) groups by trivalent or divalent heteroatoms, respectively, in such a way as to maintain the continuous  $\pi$ -electron system characteristic of aromatic systems and a number of out-of-plane  $\pi$ -electrons corresponding to the Hückel rule (4n + 2); an alternative term is hetarenes. *Comprehensive Heterocyclic Chemistry*, Vol. 1, Ed. O. Meth-Cohn, Pergamon, 1984, p. 3. *E.g.* 

# heteroaryl groups:

The class of heterocyclyl groups derived from heteroarenes by removal of a hydrogen atom from any ring atom: an alternative term is hetaryl. E.g.

atom; an alternative term is hetaryl. *E.g.*2-pyridyl (pyridin-2-yl), indol-1-yl.

# heteroarynes:

Compounds derived from heteroarenes by replacement of a formal carbon-carbon double bond by a formal triple bond (with loss of two hydrogen atoms). Also known as hetarynes and as 1,2-didehydroheteroarenes. See arynes. H. J. den Hertog and H. C. van der Plas, in Advances in Heterocyclic Chemistry, Ed. A. R. Katritzky, Vol. 4, Academic Press, 1965, p. 121. E.g.

#### heterocumulenes:

Cumulenes in which one or more carbon atoms of the cumulative bond system have been replaced by heteroatoms. E.g. O=C=C=C=O, but not CH<sub>2</sub>=C=O, ketene, nor O=C=O, carbon dioxide, which are heteroallenes.

### heterocyclic compounds:

Cyclic compounds having as ring members atoms of at least two different elements. E.g. quinoline, 1,2-thiazole, bicyclo[3.3.1]tetrasiloxane. Cf. homocyclic compounds, carbocyclic compounds.

#### heterocyclyl groups:

Univalent groups formed by removing a hydrogen atom from any ring atom of a heterocyclic compound.

E.g. 4-pyridyl, pyrrolidin-1-yl, pyrrolidin-2-yl. See organyl.

# homocyclic compounds:

Cyclic compounds having as ring members atoms of the same element only. E.g. benzene, pentazole, cyclohexasilane.

# hydrazides:\*

Compounds derived from oxoacids  $R_k E(=0)_l (OH)_m (l \neq 0)$  by replacing -OH by -NRNR<sub>2</sub> (R groups are commonly H), as in carbohydrazides, RC(=0)NHNH<sub>2</sub>, NOC Rule C-921.5, (GNOC Recom. R-5.7.8.4),

# silasesquioxanes:\*

Compounds in which every silicon atom is linked to three oxygen atoms and every oxygen atom is linked to two silicon atoms, and having the general formula  $(SiH)_{2n}O_{3n}$ . NOC Rule D-6.61. By extension hydrocarbyl derivatives are commonly included.

#### silasesquithianes:\*

Compounds in which every silicon atom is linked to three sulfur atoms and every sulfur atom is linked to two silicon atoms, and having the general formula  $(SiH)_{2n}S_{3n}$ . NOC Rule D-6.61. By extension hydrocarbyl derivatives are commonly included.

#### silathianes:\*

Compounds having the structure  $H_3Si[SSiH_2]_nSSiH_3$  and branched-chain analogues. They are analogous in structure to *siloxanes* with -S- replacing -O-. NOC Rule D-6.31. By extension *hydrocarbyl* derivatives are commonly included.

#### silazanes:\*

Saturated silicon-nitrogen hydrides, having straight or branched chains. They are analogous in structure to siloxanes with -NH- replacing -O-. NOC Rule D-6.41. E.g. H<sub>3</sub>SiNHSiH<sub>2</sub>NHSiH<sub>3</sub> trisilazane. By extension hydrocarbyl derivatives are commonly included.

#### silicones:

Polymeric or oligomeric siloxanes, usually considered unbranched, of general formula  $[-OSiR_2-]_n$  (R  $\neq$  H).

#### siloxanes:\*

Saturated silicon-oxygen hydrides with unbranched or branched chains of alternating silicon and oxygen atoms (each silicon atom is separated from its nearest silicon neighbours by single oxygen atoms). The general structure of unbranched siloxanes is  $H_3Si[OSiH_2]_nOSiH_3$ . See also silicones. NOC Rule D-6.21.  $H_3Si[OSiH_2]_nOSiH_2OSiH_3]_2$  is an example of a branched siloxane. By extension hydrocarbyl derivatives are commonly included.

#### silyl groups:

- 1. In a strict sense, the silyl group is H<sub>3</sub>Si-. NOC Rule D-6.12.
- 2. A name commonly applied to hydrocarbyl derivatives of the silyl group: R<sub>3</sub>Si-.

# silyl radicals:

- 1. In a strict sense, the silyl radical is H<sub>3</sub>Si. NOC Rule D-5.81.
- 2. A name commonly applied to the silicon-centered radicals: R<sub>3</sub>Si\*.

#### silylenes:\*

Carbene analogues having the structure R<sub>2</sub>Si:. RNRI Rule RC-81.1.3.1.

# spiro compounds:

Compounds having one atom (usually a quaternary carbon) as the only common member of two rings. NOC Rule A-41. *E.g.* spiro[cyclopentane-1,2'-indene], spiro[4.4]nonane

#### stannoxanes:

Compounds having the structure  $H_3Sn[OSnH_2]_nOSnH_3$ . Thus tin analogues of siloxanes.

stannylenes: See stannylidenes.

#### stannylidenes:\*

Carbene analogues having the structure R<sub>2</sub>Sn: The older synonymous term stannylenes is no longer recommended, RNRI Rule RC-81.1.3.2.