

A Guide to
IUPAC Nomenclature
of Organic Compounds
Recommendations 1993

International Union of Pure and Applied Chemistry
Organic Chemistry Division
Commission on Nomenclature of Organic Chemistry (III.1)

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IUPAC Nomenclature
of Organic Compounds
Recommendations 1993**

(including revisions, published and hitherto unpublished, to the
1979 edition of *Nomenclature of Organic Chemistry*)

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R-2 Parent Hydrides¹⁸ and their Derived Substituent Groups

R-2.0 INTRODUCTION

A 'parent hydride' (see R-0.2.1.1) is the structure which is named before the addition of affixes denoting substituents to yield the name of a specific compound. Its name is understood to signify a definite population of hydrogen atoms attached to a skeletal structure. Acyclic parent hydrides are always unbranched, for example pentane and trisilane; although a few trivial names for branched acyclic hydrocarbons are retained (see R-9.1, Table 19(a), p. 163), their use for naming substitutive derivatives is not recommended. Cyclic parent hydrides are usually either fully saturated, for example, cyclopentane, cyclotrisiloxane, azepane, bicyclo[2.2.2]octane, and spiro[4.5]decane, or fully unsaturated, i.e., they contain the maximum number of noncumulative double bonds, for example, pyridine, 1,3-oxazole, 1*H*-phenalene, phenanthroline, and benzo[*a*]-anthracene. Also, there are parent hydrides that are partially saturated, for example, 1,4-dihydro-1,4-ethanoanthracene and spiro[1,3-dioxolane-2,1'-[1*H*]indene], and that are combinations of cyclic and saturated acyclic structures having retained trivial names (see R-9.1, Table 19(a), p. 163).

R-2.1 MONONUCLEAR HYDRIDES

The names of mononuclear hydrides of the elements for use as parents in substitutive nomenclature are given in Table 2. Many are formed systematically by combining the 'a' term of the element (with elision of the terminal 'a') with the ending '-ane', for example, borane for BH_3 , silane for SiH_4 , etc. There are important exceptions: methane for CH_4 , oxidane for OH_2 , sulfane for SH_2 , selenane for SeH_2 , etc., (see Table 2). The systematic alternatives to well established common names, e.g., azane for ammonia, oxidane for water, and chlorane, bromane, etc., for hydrogen chloride, bromide, etc., are necessary for naming some derivatives and for generating names of polynuclear homologues. If the bonding number of the element differs from the normal one as defined in R-1.1, the name of the hydride is modified by affixing a *z* symbol as instructed by R-1.1.

R-2.2 ACYCLIC POLYNUCLEAR HYDRIDES

R-2.2.1 Hydrocarbons

The saturated unbranched acyclic hydrocarbons from C_2 to C_4 are named ethane, propane, and butane (see R-9.1, Table 19(a), p. 162). Systematic names of the higher members of this series consist of a numerical term (see Table 11, p. 71), followed by '-ane' with elision of a terminal 'a' from the basic numerical term. The generic name for saturated acyclic hydrocarbons (branched or unbranched) is 'alkane'. The chain is numbered from one end to the other with arabic numerals.

¹⁸ More detailed recommendations for naming these compounds are given in Sections A, B, and D of the 1979 edition of the IUPAC *Nomenclature of Organic Chemistry*¹.

Table 2 Mononuclear hydrides

BH ₃	Borane ^a	OH ₂	Oxidane ^{c,e,f}
CH ₄	Methane ^b (Carbane)	SH ₂	Sulfane ^{c,f}
SiH ₄	Silane	SH ₄	λ^4 -Sulfane ^{c,g}
GeH ₄	Germane	SH ₆	λ^6 -Sulfane ^{c,g}
SnH ₄	Stannane	SeH ₂	Selane ^{c,f,g}
PbH ₄	Plumbane	TeH ₂	Tellane ^{c,f}
NH ₃	Azane ^{c,d}	PoH ₂	Polane ^{c,f}
PH ₃	Phosphane ^b (Phosphine)	FH	Fluorane ^{c,f}
PH ₅	λ^5 -Phosphane ^b (Phosphorane)	ClH	Chlorane ^{c,f}
AsH ₃	Arsane ^b (Arsine)	BrH	Bromane ^{c,f}
AsH ₅	λ^5 -Arsane ^b (Arsorane)	IH	Iodane ^{c,f}
SbH ₃	Stibane ^b (Stibine)	IH ₃	λ^3 -Iodane ^h
SbH ₅	λ^5 -Stibane ^b (Stiborane)	IH ₅	λ^5 -Iodane ^g
BiH ₃	Bismuthane ^{b,c} (Bismuthine)	AtH	Astatane ^f

^a Although analogous names have been suggested for aluminium and gallium hydrides, they are not included in these recommendations.

^b Preferred name.

'Ammonia', 'water', 'hydrogen chloride' (and analogues) are common names for NH_3 , OH_2 , and ClH (and analogues), respectively.

^dThe name amine is used, for example, in *Beilstein*, as a parent hydride name for NH_3 .

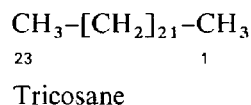
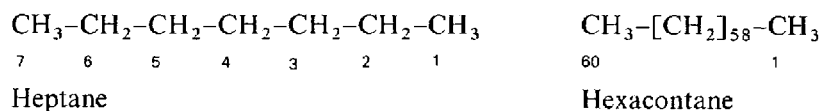
^e Exceptions. The expected names, bismane, oxane, thiane, selenane, tellurane and polonane are Hantzsch-Widman names for heteromonocyclic rings (see R-2.3.3).

[†] The normal formulae H₂O, H₂S, etc., have been reversed in this table for the purpose of comparison.

⁶The names 'sulfurane' and 'selenurane', and related names, such as persulfurane and periodinane, which have been used in recent literature, are not recommended.

^b The name 'iodinane', which has been used in recent literature, cannot be used because it is a Hantzsch-Widman name for a heteromonocyclic iodine ring (see R-2.3.3).

Examples:



R-2.2.2 Homogeneous hydrides other than hydrocarbons or boron hydrides¹⁹

A compound consisting of an unbranched chain containing several identical heteroatoms saturated with hydrogen atoms, may be named by citing the appropriate multiplying prefix (with *no elision* of the terminal vowel of the multiplying prefix) followed by the appropriate name of the hydride according to R-2.1. If necessary, a λ^n symbol is used, according to R-1.1.

¹⁹ Polyboranes are not covered in these recommendations; because of their unique bonding characteristics, they have been treated in IUPAC *Nomenclature of Inorganic Chemistry*³, Recommendations I-11.1 through I-11.3, pp. 207–225.

Table 11 Basic numerical terms (multiplying affixes)⁵¹

Number	Numerical term	Number	Numerical term	Number	Numerical term	Number	Numerical term
1	mono- ^a	11	undeca-	100	hecta-	1000	kilia-
2	di- ^a	12	dodeca- ^b	200	dicta-	2000	dilia-
3	tri-	20	icosa- ^c	300	tricta-	3000	trilia-
4	tetra-	30	triaconta-	400	tetracta-	4000	tetralia-
5	penta-	40	tetraconta-	500	pentacta-	5000	pentalia-
6	hexa-	50	pentaconta-	600	hexacta-	6000	hexalia-
7	hepta-	60	hexaconta-	700	heptacta-	7000	heptalia-
8	octa-	70	heptaconta-	800	octacta-	8000	octalia-
9	nona-	80	octaconta-	900	nonacta-	9000	nonalia-
10	deca-	90	nonaconta-				

^aWhen alone, the numerical term for the number 1 is 'mono-' and that for 2 is 'di-'. In association with other numerical terms, the number 1 is represented by 'hen-' (except in the case of 'undeca-') and the number 2 by 'do-' (except in the cases of 'dicta-' and 'dilia-'). The numerical term for the number 11 is 'undeca-'. Compare *monochloro* with *henicosane* for the number 21 and *dichloro* with *docosane* for the number 22.

^bAfter 'dodeca-' (12), composite numerical terms are formed systematically by citing the basic terms in the order opposite to that of the constituent arabic numerals. For example, the numerical term for the number 468 is 'octahexacontatetracta-'.

^cChemical Abstracts Service and *Beilstein* use *eicosa* instead of *icosa*.

The basic numerical terms (multiplying affixes) given in Table 11 are used by direct joining without hyphen.

Numerical terms for use as multiplying prefixes for complex entities, such as substituted substituents, are obtained by adding the ending '-kis' to the numerical term defined as above. However, the ending '-kis' is not used with 'mono-'. As exceptions, 'bis-' is used for the number 2 and 'tris-' for 3.

Examples:

4 tetrakis-
231 hentriacontadictakis-

The following multiplying prefixes are used in names for unbranched assemblies of three or more identical repeating units.

2	bi-	5	quinque-	8	octi-
3	ter-	6	sexi-	9	novi-
4	quater-	7	septi-	10	deci-

When a substituent is itself substituted (a complex substituent, see R-4.2.4), all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituents is regarded as a 'parent substituent' (analogous to a parent hydride). The nomenclature of the whole substituent is subject to all the procedures adopted for

⁵¹International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, 'Extension of Rules A-1.1 and A-2.5 Concerning Numerical Terms Used in Organic Nomenclature (Recommendations 1986)', *Pure Appl. Chem.*, **58**, 1693-1696 (1986).