CHAPTER P-4 RULES FOR NAME CONSTRUCTION

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P-40 Introduction

In this Chapter, principles regarding name construction are presented. It is recognized that in chemical discussions it may sometimes be convenient to depart from rigorous rules in order to provide a name more appropriate to the chemical intent or to avoid obscuring an important feature. However, such deviations should not be done without good reason, and names so derived are not recommended for general use in publications.

The application of the principles and rules described in this Chapter has been devised to lead to a preferred IUPAC name. Preferred IUPAC names are not necessarily the aim of a practicing chemist who wants to communicate with his colleagues in familiar, well understood terms, but it may be appropriate to those who cite chemical names in legislative documents, in international trade and commerce, or for preparing programs for index purposes, databases and retrieval systems.

This Chapter includes the general rules and orders of seniority used in substitutive nomenclature and functional class nomenclature.

P-41 Order of seniority of classes

The order of seniority of classes is given in Table 4-1. It ranks classes expressed by suffixes (classes 1 through 20) and classes based on the senior atom in compounds (classes 21 to 35).

Table 4.1 General compound classes listed in decreasing order of seniority for choosing and naming the principal class (radicals and ions) or characteristic group in an organic compound*

Ionic classes

- 1 Radicals
- 2 Radical anions
- 3 Radical cations
- Anions
- 5 Zwitterions
- Cations

Classes expressed by characteristic groups

- 7 Acids.
 - 7a 'Suffix' acids in the order carboxylic (not including carbonic, oxalic, or polycarbonic acids, which belong to sub-class '7b'), sulfonic, sulfinic, selenonic, seleninic, telluronic, tellurinic, each followed in turn by the corresponding peroxy, imidic, and hydrazonic acids. Chalcogen analogues follow each of the corresponding oxygen acids and, in each case, the chalcogen analogue with the greater number of the preferred chalcogen atom (O > S > Se > Te), considered first in -OOH groups, then in -OH groups as necessary. (See P-42 for the complete list of seniority of acids, P-43 for suffixes modified by functional replacement, and Appendix 1 for an extensive list of the order of seniority of these suffixes).
 - 7b Carbon acids with no substitutable hydrogen atoms in the order polynuclear carbonic acids (tricarbonic acid, dicarbonic acid), then oxalic acid, and carbonic acid
 - 7c Oxoacids having substitutable hydrogen atoms attached to their central atoms and their acidic derivatives in the following decreasing order of seniority: azonic, azinic, phosphonic, phosphinous acids, etc. (see P-42 for the complete list).
 - 7d Mononuclear and polynuclear oxoacids other than carbon acids without substitutable hydrogen atoms attached to their central atom (see 7b, above), but that may be functionalized or may form derivatives by functional replacement having substitutable hydrogen atoms.
 - 7e Other monobasic 'oxo acids' used as functional parent compounds.
- 8 Anhydrides [substitutive nomenclature is used for cyclic anhydrides (see 16 below); functional class names are given to acyclic anhydrides and to a few cyclic anhydrides corresponding to acids having retained names; cyclic anhydrides are preferred over noncyclic anhydrides, when functional names are used].
- 9 Esters (functional class names are given to noncyclic esters; lactones and other cyclic esters are named as heterocycles; see 16 below).
- 10 Acid halides and pseudohalides [first in the order of the corresponding acid given above, then in the order of the halogen atoms (-F > -Cl > -Br > -I); then in the following order of pseudohalogen groups ($-N_3 > -CN > -NC > -NCO > -NCS > -NCSe > -NCTe > -CNO$).
- 11 Amides [in the order of the corresponding acids; cyclic amides are named as heterocycles (see 16 below)].
- 12 Hydrazides (in the order of corresponding acids).
- 13 Imides (includes only cyclic imides derived from organic di- or polybasic acids having retained names).
- 14 Nitriles.
- 15 Aldehydes and chalcogen analogues.
- 16 Ketones (of the type -C-CO-C-), pseudoketones (of the type -C-CO-X, X-CO-X, or -CO-X-CO-, where $X \neq C$, halogen, pseudohalogen, or NH₂) and heterones. See Classes 8, 9 and 10, on lactones, lactams, anhydrides, imides.

- 17 Hydroxy compounds and chalcogen analogues (includes alcohols and phenols, which no longer have a separate ranking order).
- 18 Hydroperoxides (peroxols), i.e., -OOH.
- 19 Amines (defined as having three single covalent attachments to a nitrogen atom, i.e., NR₃).
- 20 Imines, R=NH or R=N-R'.

Classes denoted by the senior atom in heterane nomenclature

- 21 Nitrogen compounds: heterocycles, polyazanes, hydrazines (except for hydrazides), diazenes, hydroxylamines, azanes (except for amides and amines)
- 22 Phosphorus compounds: heterocycles, polyphosphanes, phosphanes
- 23 Arsenic compounds: heterocycles, polyarsanes, arsanes
- 24 Antimony compounds: heterocycles, polystibanes, stibanes
- 25 Bismuth compounds: heterocycles, polybismuthanes, bismuthanes
- 26 Silicon compounds: heterocycles, polysilanes, silanes
- 27 Germanium compounds: heterocycles, polygermanes, germanes
- 28 Tin compounds: heterocycles, polystannanes, stannanes
- 29 Lead compounds: heterocycles, polyplumbanes, plumbanes
- 30 Boron compounds: heterocycles, polyboranes, boranes
- 31 Aluminium compounds: heterocycles, polyalumanes, alumanes
- 32 Gallium compounds: heterocycles, polygallanes, gallanes
- 33 Indium compounds: heterocycles, polyindiganes, indiganes
- 34 Thallium compounds: heterocycles, polythallanes, thallanes
- 35 Oxygen compounds: heterocycles, polyoxidanes (trioxidane but not peroxides or ethers)
- 36 Sulfur compounds: heterocycles, polysulfanes (trisulfane, λ^4 and λ^6 mono and disulfanes, but not disulfides or sulfides)
- 37 Selenium compounds: heterocycles, polyselanes (triselane but not diselenides, selenides)
- 38 Tellurium compounds: heterocycles, polytellanes (tritellane but not ditellurides, tellurides)
- 39 λ^3 , λ^5 , and λ^7 halogen compounds in the order F > Cl > Br > I.
- 40 Carbon compounds: rings, chains
- 41 λ^1 Halogen compounds in the order F > Cl > Br > I

* In this table, the the symbol '>' means 'is senior to'.

Examples:

HOOC-CH₂-CH₂-2-carboxyethyl (PIN) [free valence (radical) > carboxylic acid]

HO-CH₂-CH₂-CONH₂

3-hydroxypropanamide (PIN) (amide > alcohol) OHC-CH₂-CH₂-CN

 $(CH_3)_3N^+-CH_2-COO^-$

(anion > cation)

(trimethylazaniumyl)acetate (PIN)

4-oxobutanenitrile (PIN) (nitrile > aldehyde)

HSSS-SiH₃

trisulfanylsilane (preselected name, see P-12.2) (Si > S)

BH₂-PH₂

boranylphosphane (preselected name, see P-12.2) (P > B)

(CH₃)₄Si tetramethylsilane (PIN) (Si > C)

triphenylphosphane (PIN) (P > C)

 $(C_{6}H_{5})_{3}P$

P-42 Order of seniority of acids and derivatives

Acids of class 7 (see Table 4.1) in the order of classes of compounds are further classified into subclasses. They correspond to acids expressed by suffixes and acids used as functional parents (see P-34). The following subsections complete the brief description given in Class 7; the acids are described in decreasing seniority order.

P-42.1 Class 7a. Acids expressed by suffixes (excludes carbonic, oxalic, and polycarbonic acids)

carboxylic acids	-соон -(С)(О)ОН	-carboxylic acid -oic acid
sulfonic acids	-SO ₂ -OH	-sulfonic acid
sulfinic acids	-SO-OH	-sulfinic acid
selenonic acids	-SeO ₂ -OH	-selenonic acid
seleninic acids	-SeO-OH	-seleninic acid
telluronic acids	-TeO ₂ -OH	-telluronic acid
tellurinic acids	-TeO-OH	-tellurinic acid

P-42.2 Class 7b. Carbon acids with no substitutable hydrogen atoms

polycarbonic acids dicarbonic acid oxalic acid carbonic acid cyanic acid

P-42.3 Class 7c. Noncarbon acids having substitutable hydrogen atoms on the central atom.

All these names are preselected names. In this class, criteria for seniority are, in descending order:

5

- (a) the central atom first in the list N > P > As > Sb > B;
- (b) maximum number of central atoms;
- (c) homopolyacids (isopolyacids) (see ref. 14);
- (d) having contiguous central atoms;
- (e) maximum number of acidic (-OH) groups;
- (f) highest oxidation number for the central atom

azonic acid	NH(O)(OH) ₂
azinic acid	NH ₂ (O)(OH)
polyphosphonic acids	$(\mathrm{HO})\mathrm{PH}(\mathrm{O})\text{-}\mathrm{O}\text{-}[\mathrm{PH}(\mathrm{O})\text{-}\mathrm{O}\text{-}]_{n}\mathrm{PH}(\mathrm{O})(\mathrm{OH})$
diphosphonic acid	(HO)PH(O)-O-PH(O)(OH)
hypodiphosphonic acid (see P-67.2.1)	(HO)(O)HP-PH(O)(OH)
phosphonic acid	PH(O)(OH) ₂
polyphosphonous acids	(HO)PH-O-[PH-O-] _n PH(OH)
diphosphonous acid	(HO)PH-O-PH(OH)
hypodiphosphonous acid (see P-67.2.1)	(HO)HP-PH(OH)
phosphonous acid	PH(OH) ₂
phosphinic acid	PH ₂ (O)(OH)
phosphinous acid	PH ₂ (OH)
polyarsonic acids > diarsonic acid > hypodiar	sonic acid (see P-67.2.1)
arsonic acid	AsH(O)(OH) ₂
polyarsonous acids > diarsonous acid > hypot	diarsonous acid (see P-67.2.1)
arsonous acid	AsH(OH) ₂
arsinic acid	AsH ₂ (O)(OH)

arsinous acid	AsH ₂ (OH)
polystibonic acids > distibonic acid > hypodia	stibonic acid (see P-67.2.1)
stibonic acid	SbH(O)(OH) ₂
polystibonous acids > distibonous acid > hyp	odistibonous acid (see P-67.2.1)
stibonous acid	SbH(OH) ₂
stibinic acid	SbH ₂ (O)(OH)
stibinous acid	SbH ₂ (OH)
diboronic acid	(HO)BH-O-BH-(OH)
hypodiboronic acid (see P-67.2.1)	(HO)HB-BH(OH)
boronic acid	BH(OH) ₂
borinic acid	BH ₂ (OH)

P-42.4 Class 7d. Noncarbon acids used to generate derivatives having substitutable hydrogen atoms. All these names are preselected names. In this class, criteria for seniority are, in descending order:

(a) the central atom first in the list: P > As > Sb > Si > B > S > Se > Te;

- (b) maximum number of central atoms;
- (c) homopolyacids (isopolyacids) (see ref. 14);
- (d) polyacids having contiguous central atoms;
- (e) maximum number of acidic groups (-OH) groups);
- (f) highest oxidation number for the central atom.

For consistency in the names of polynuclear oxoacids, the numerical infix 'di' has been uniformly used in naming dinuclear 'hypo' acids, for example, hypodiphosphorous acid, rather than hypophosphorus acid.

polyphosphorous acids	(HO) ₂ P-O-	$[P(OH)-O]_n - P(OH)_2$
tetraphosphoric acid	$(HO)_2P(O)$	$O-P(O)(OH)-O-P(O)(OH)-O-P(O)(OH)_2$
triphosphoric acid	$(HO)_2P(O)$	-O-P(O)(OH)-O-P(O)(OH) ₂
diphosphoric acid	(HO) ₂ P(O)-	-O-P(O)(OH) ₂
diphosphorous acid	(HO) ₂ P-O-	P(OH) ₂
hypodiphosphoric acid (see l	P-67.2.1)	(HO) ₂ (O)P-P(O)(OH) ₂
hypodiphosphorous acid (see	e P-67.2.1)	(HO) ₂ P-P(OH) ₂
phosphoric acid		P(O)(OH) ₃
phosphorous acid		P(OH) ₃

polyarsoric acids > polyarsorous acids > diarsoric acid > diarsorous acid > hypodiarsoric acid (see P-67.2.1) > hypodiarsorous acid (see P-67.2.1)

	arsoric acid	As(O)(OH) ₃		
	arsorous acid	As(OH) ₃		
	polystiboric acids > polystibonous acid acid (see P-67.2.1) > hypodist	d > distiboric acid > distibonous acid > hypodistiboric ibonous acid (see P-67.2.1)		
	stiboric acid	Sb(O)(OH) ₃		
	stiborous acid	Sb(OH) ₃		
	orthosilicic acid	Si(OH) ₄		
	diboric acid	(HO) ₂ B-O-B(OH) ₂		
	hypodiboric acid (see P-67.2.1)	(HO) ₂ B-B(OH) ₂		
	boric acid	B(OH) ₃		
	polysulfuric acids	(HO)SO ₂ -O-[SO ₂ (OH)-O-] _n SO ₂ (OH)		
	polysulfurous acids	(HO)SO-O-[SO(OH)-O-] $_n$ SO(OH)		
	disulfuric acid	(HO)SO ₂ -O-SO ₂ (OH)		
	disulfurous acid	(HO)S(O)-O-S(O)(OH)		
	dithionic acid (hypodisulfuric acid)	$(HO)O_2S-SO_2(OH)$		
	dithionous acid (hypodisulfurous acid)	(HO)(O)S-S(O)(OH)		
	sulfuric acid	S(O) ₂ (OH) ₂		
	sulfurous acid	S(O)(OH) ₂		
	polyselenic acids > polyselenous acids hypodiselenic acid (see P-67.2.	 > diselenic acid > diselenous acid > 1) > hypodiselenous acid (see P-67.2.1) 		
	selenic acid	Se(O) ₂ (OH) ₂		
	selenous acid	Se(O)(OH) ₂		
		 s > ditelluric acid > ditellurous acid > 1) > hypoditellurous acid (see P-67.2.1) 		
	telluric acid	$Te(O)_2(OH)_2$		
	tellurous acid	$Te(O)(OH)_2$		
		o' acids used as functional parents. All these names for seniority are, in descending order.		
-				

(a) the central atom first in the list $N > Cl > Br > I$;
(b) highest oxidation number for the central atom.

nitric acid	HO-NO ₂
nitrous acid	HO-NO
perfluoric acid	F(O) ₃ OH
fluoric acid	F(O) ₂ OH

fluorous acid	F(O)OH
hypofluorous acid	FOH
perchloric acid	Cl(O) ₃ OH
chloric acid	Cl(O) ₂ OH
chlorous acid	Cl(O)OH
hypochlorous acid	ClOH
perbromic acid	Br(O) ₃ OH
bromic acid	Br(O) ₂ OH
bromous acid	Br(O)OH
hypobromous acid	BrOH
periodic acid	$I(O)_3OH$
iodic acid	$I(O)_2OH$
iodous acid	I(O)OH
hypoiodous	IOH

P-43 Order of seniority of suffixes

P-43.0 Introduction

The order of seniority for suffixes is described in this Section. It is based on the seniority of classes 7 through 20 given in Table 4.1 and includes suffixes modified by functional replacement.

P-43.1 General methodology of functional replacement

Suffixes are modified as indicated in Table 4.3. Prefixes and infixes are used as indicated in Table 4.2. Prefixes are used to modify suffixes such as 'ol', 'al', for example 'thiol' and 'thial'. Infixes are recommended to modify the suffixes 'carboxylic acid', 'sulfonic acid', and related suffixes, for example 'carboperoxoic acid' and 'sulfonothioic acid'.

Table 4.2 Prefixes and infixes, in decreasing order of seniority, used to generate suffixes in preferred IUPAC names by functional replacement

 Prefix	Infix	Replaced atom(s)	Replacing atom(s)
peroxy-	-peroxo-	-0-	-00-
thioperoxy-	-(thioperoxo)-	-0-	-OS- or -SO-
dithioperoxy-	-(dithioperoxo)-	-0-	-SS-
thio-	-thio-	-O- or =O	-S- or $=S$
seleno-	-seleno-	-O- or $=O$	-Se- or $=Se$

telluro-	-telluro-	-O- or $=O$	-Te- or =Te	
imido-	-imido-	=O	=NH	5
hydrazono-	-hydrazono-	=O	=NNH ₂	~

When several oxygen atoms are replaceable, the following criteria are applied, in order, until a decision is reached:

9

- (a) maximum number of oxygen atoms, then S, Se, and Te atoms, then =NH and =NNH₂ groups;
- (b) maximum number of oxygen atoms, then S, Se, and Te atoms, in -OO- groups;
- (c) oxygen atoms, then S, Se and Te atoms, in –(O)OH and –OH groups.

The order of seniority is described, in the case of carboxylic acids, sulfonic acids and sulfinic acids, by indicating, after the name of the modified suffix the number and kind of atoms used in the replacement operation (see Table 4.2).

Table 4.3 gives the list, in decreasing order, of the seniority of suffixes and suffixes modified by functional replacement for carboxylic and sulfonic acids. Sulfinic acid suffixes are similar to sulfonic acids. Selenium and tellurinum acid suffixes are formed by replacing 'sulf' by 'selen' or 'tellur'.

Table 4.3 Carboxylic and sulfonic acid suffixes generated for IUPAC preferred names by functional replacement, in decreasing order of seniority

1 Carboxylic acids

-СООН	carboxylic acid	
-СО-ООН	carboperoxoic acid	(30)
-CS-OOH	carboperoxothioic OO-acid	(20,1S; 00)
-CSe-OOH	carboperoxoselenoic acid	(20,1Se; OO)
-CO-SOH	carbo(thioperoxoic) SO-acid	(2O,1S; OS; OH)
-CO-OSH	carbo(thioperoxoic) OS-acid	(2O,1S; OS; SH)
-CO-SeOH	carbo(selenoperoxoic) SeO-acid	(2O,1Se; OSe; OH)
–CO-OSeH	carbo(selenoperoxoic) OSe-acid	(20,1Se; OSe; SeH)
-CS-SOH	carbothio(thioperoxoic) SO-acid	(10,2S; OS; OH)
-CS-OSH	carbothio(thioperoxoic) OS-acid	(10,2S; OS; SH)
-CSe-OSH	carboseleno(thioperoxoic) OS-acid	(10,1S,1Se; OS; SH)
-CS-SeOH	carbo(selenoperoxo)thioic SeO-acid	(10,1S,1Se; OSe: OH)
-CS-OSeH	carbo(selenoperoxo)thioic OSe-acid	(10,1S,1Se; OSe; eH)
-CS-SSH	carbo(dithioperoxo)thioic acid	(3S)

-CSe-SeSeH	carbo(diselenoperoxo)selenoic acid	(3Se)
–СТе-ТеТеН	carbo(ditelluroperoxo)telluroic acid	(3Te)
-CS-OH	carbothioic O-acid	(10,1S; OH)
-CO-SH	carbothioic S-acid	(10,1S; SH)
-CS-SH	carbodithioic acid	(2S)
-CSe-SH	carboselenothioic S-acid	(1S,1Se; SH)
-CS-SeH	carboselenothioic Se-acid	(1S,1Se; SeH)
-CSe-SeH	carbodiselenoic acid	(2Se)
-CTe-SeH	carboselenotelluroic Se-acid	(1Se,1Te; SeH
–СТе-ТеН	carboditelluroic acid	(2Te)
-C(=NH)-OH	carboximidic acid	
-C(=NH)-OOH	carbimidoperoxoic acid	(20,1N; OO)
-C(=NH)-SOH	carbimido(thioperoxoic) SO-acid	(10,1S,1N; OS; OH)
-C=(NH)-OSH	carbimido(thioperoxoic) OS-acid	(10,1S,1N; OS; SH)
-C(=NH)-SSH	carbo(dithioperox)imidic acid	(2S,1N; SS)
-C(=NH)-SeSH	carbimido(selenothioperoxoic) SeS-acid	(1S,1Se,1N; SSe; SH)
-C(=NH)-SH	carbimidothioic acid	(1S,1N)
-C(=NH)-SeH	carbimidoselenoic acid	(1Se,1N)
-C(=NH)-TeH	carbimidotelluroic acid	(1Te,1N)
-C(=NNH ₂)-OH	carbohydrazonic acid	
-C(=NNH ₂)-OOH	carbohydrazonoperoxoic acid	(20,1NN; OO)
-C(=NNH ₂)-SOH	carbohydrazono(thioperoxoic) SO-acid	(10,1S,1NN; OS; OH)
-C(=NNH ₂)-OSH	carbohydrazono(thioperoxoic) OS-acid	(10,1S,1NN; OS; SH)
-C(=NNH ₂)-TeTeH	Carbo(ditelluroperoxo)hydrazonoic acid	(2Te,1NN; TeTe)

2 Sulfonic acids

	–SO ₂ -OH sulfonic acid			
	-SO ₂ -OOH	sulfonoperoxoic acid	(40)	
	-S(O)(S)-OOH	sulfonoperoxothioic OO-acid	(30,1S; OO)	
	-S(O)(Se)-OOH	sulfonoperoxoselenoic OO-acid	(30,1Se; OO)	
	-SO ₂ -SOH	sulfono(thioperoxoic) SO-acid	(30,1S; OS; OH)	
\sim	-SO ₂ -OSH	sulfono(thioperoxoic) OS-acid	(30,1S; OS; SH)	
	-SS ₂ -OOH	sulfonoperoxodithioic OO-acid	(2O,2S; OO)	

-S(O)(S)-SOH	sulfonothio(thioperoxoic) SO-acid	(20,2S; OS; OH)
-S(S)(Se)-OOH	sulfonoperoxoselenothioic OO-acid	(20,1S,1Se; 00)
-SSeSe-SSH	sulfino(dithioperoxo)diselenoic acid	(2S,2Se; SS)
-SS ₂ -SeSeH	sulfono(diselenoperoxo)dithioic acid	(2S,2Se; SeSe)
-STe ₂ -TeTeH	sulfono(ditelluroperoxo)ditelluroic acid	(4Te)
-S(O)(S)-OH	sulfonothioic O-acid	(2O,1S; OH)
-SO ₂ -SH	sulfonothioic S-acid	(2O,1S; SH)
-SO ₂ -SeH	sulfonoselenoic Se-acid	(2O,1Se; SeH)
-SS ₂ -OH	sulfonodithioic O-acid	(10,2S; OH)
-S(O)(S)-SH	sulfonodithioic S-acid	(10,2S; SH)
-S(Se)(Te)-OH	sulfonoselenotelluroic O-acid	(10,1Se,1Te; OH
-S(O)(Te)-SeH	sulfonoselenotelluroic Se-acid	(10,1Se,1Te; SeH)
-S(O)(Se)-TeH	sulfonoselenotelluroic <i>Te</i> -acid	(10,1Se.1Te; TeH)
-SS ₂ -SH	sulfonotrithioic acid	(38)
-S(O)(=NH)-OH	sulfonimidic acid	
-S(O)(=NH)-OOH	sulfonimidoperoxoic acid	(30,1N; OO)
-S(S)(=NH)-OOH	sulfonimidoperoxothioic OO-acid	(20,1S,1N; OO; OH)
-S(O)(=NH)-SOH	sulfonimido(thioperoxoic) OO-acid	(20,1S,1N; OS; OH)
-S(O)(=NH)-OSH	sulfonimido(thioperoxoic) OS-acid	(20,1S,1N; OS; SH)
-S(S)(=NH)-OH	sulfonimidothioic O-acid	(10,1S; OH)
-S(O)(=NH)-SH	sulfonimidothioic S-acid	(10,1S; SH)
-S(S)(=NH)-SH	sulfoimidodithioic acid	(28)
-S(Se)(=NH)-SH	sulfonimidoselenothioic S-acid	(1S,1Se; SH)
-S(S)(=NH)-SeH	sulfonimidoselenothioic Se-acid	(1S,1Se; SeH)
-S(Te)(=NH)-TeH	sulfonimidoditelluroic acid	(2Te)
-S(=NH) ₂ -OH	sulfonodiimidic acid	
-S(=NH) ₂ -OOH	sulfonodiimidoperoxoic acid	(20,2N; OO)
-S(=NH) ₂ -SOH	sulfonodiimido(thioperoxoic) SO-acid	(10,1S,2N: OS; OH)
-S(=NH) ₂ -OSH	sulfonodiimido(thioperoxoic) OS-acid	(10,1S,2N; OS; SH)
-S(=NH) ₂ -SeH	sulfonodiimidoselenoic acid	(1Se,2N)
-S(=NH) ₂ -TeH	sulfonodiimidotelluroic acid	(1Te,2N)
-S(O)(=NNH ₂)-OH	sulfonohydrazonic acid	

-S(O)(=NNH ₂)-OOH	sulfonohydrazonoperoxoic acid	(30,1NN; OO)
-S(S)(=NNH ₂)-OOH	sulfonohydrazonoperoxothioic acid	(20,1S,1NN; 00)
-S(S)(=NH ₂)-OH	sulfonohydrazonothioic O-acid	(10,1S,1NN; OH)
-S(O)(=NNH ₂)-SH	sulfonohydrazonothioic S-acid	(10,1S,1NN; SH)
-S(=NNH ₂) ₂ OH	sulfonodihydrazonic acid	
-S(=NNH ₂) ₂ -OOH	sulfonodihydrazonoperoxoic acid	(20,2NN; OO)
-S(=NNH ₂) ₂ -SOH	sulfonodihydrazono(thioperoxoic) SO-acid	1 (10,1S,2NN; SO, OH)
-S(=NNH ₂) ₂ -SH	sulfonodihydrazonothioic acid	(1 S ,2NN)

Table 4.4 Complete list of suffixes and functional replacement analogues for IUPAC preferred names, in decreasing order of seniority

1. Carboxylic acids	-СО-ОН	carboxylic acid	
	-(С)О-ОН	oic acid	
Carboperoxoic acids	-СО-ООН	carboperoxoic acid	
	-(С)О-ОН	peroxoic acid	
Carboperoxoic acids modified by replacement with S, Se and/or Te			
-CS-OOH	carbopero	oxothioic acid	
–(C)S-OOH	peroxothi	oic acid	
-CSe-OOH	carbopero	oxoselenoic acid	
$-(C)Se_{-}OOH$	perovosel	enoic acid	

–(C)Se-OOH	peroxoselenoic acid
-СО-SOH	carbo(thioperoxoic) SO-acid
-(С)О-SOH	(thioperoxoic) SO-acid
–CO-OSH	carbo(thioperoxoic) OS-acid
–(C)O-OSH	(thioperoxoic) OS-acid

Carboxylic acids modified by replacement with S, Se, and/or Te

	CS-ОН (С)S-ОН	carbothioic <i>O</i> -acid thioic <i>O</i> -acid
	–CO-SH –(C)O-SH	carbothioic S-acid thioic S-acid
2^{\times}	–CO-SeH –CO-SeH	carboselenoic Se-acid selenoic Se-acid
	-CS-SH -C(S)-SH	carbodithioic acid dithioic acid

2. Carboximidic acids	-C(=NH)-OH -(C)(=NH)-OH	carboximidic acid imidic acid
Carboximidoperoxoic acids	-C(=NH)-OOH -(C)=(NH)-OOH	carboximidoperoxoic acid imidoperoxoic acid

Carboximidoperoxoic acids modified by replacement with S, Se and/or Te

-C=(NH)-SOH	carboximido(thioperoxoic) SO-acid
-(C)(=NH)-SOH	imido(thioperoxoic) SO-acid
-C(=NH)-OSH	carboximido(thioperoxoic) OS-acid
-(C)(=NH)-OSH	imido(thioperoxoic) OS-acid
-C=(NH)-SSH	carbo(dithioperox)imidic acid
-(C)(=NH)-SSH	(dithioperox)imidic acid
-C(=NH)-SeSH -(C)(=NH)-SeSH	carboximido(selenothioperoxoic) SeS-acid carboximido(selenothioperoxoic) SeS-acid

All or

Carboximidic acids modified by replacement with S, Se and/or Te

-C(=NH)-SH	carboximidothioic acid
-(C)(=NH)-SH	carboximidothioic acid

3. Carbohydrazonic acids	-C(=NNH ₂)-OH	carbohydrazonic acid
	$-(C)(=NHNH_2)$	hydrazonic acid

Carbohydrazonoperoxoic acids modified by replacement with S, Se and/or Te

-C(=NNH ₂)-SOH	carbohydrazono(thioperoxoic) SO-acid
-(C)(=NNH ₂)-SOH	hydrazono(thioperoxoic) SO-acid
-C(=NNH ₂)-OSH	carbohydrazono(thioperoxoic) OS-acid
-(C)(=NNH ₂)-OSH	hydrazono(thioperoxoic) OS-acid
−C(=NNH ₂)-TeTeH	carbo(ditelluroperoxo)hydrazonoic acid
−(C)(=NNH ₂)-TeTeH	(ditelluroperoxo)hydrazonoic acid

Carbohydrazonic acids modified by replacement with S, Se and/or Te

-C(=NHNH ₂)-SH -(C)(=NHNH ₂)-SH		carbohydrazonothioic acid carbohydrazonothioic acid
4. Sulfonic acids	-SO ₂ -OH	sulfonic acid
Sulfonoperoxoic acids	-SO ₂ -OOH	sulfonoperoxoic acid
	1 1.0.11	1

Sulfonoperoxoic acids modified by replacement with S, Se and/or Te

-S(O)(S)-OOH	sulfonoperoxothioic acid
-SO ₂ -SOH	sulfono(thioperoxoic) SO-acid

-SO ₂ -OSH	sulfono(thioperoxoic) OS-acid
-SS ₂ -OOH	sulfonoperoxodithioic acid

Sulfonic acids modified by replacement with S, Se and/or Te

-SO ₂ -SH	sulfonothioic S-acid
-S(O)(S)-OH	sulfonothioic O-acid
-S(S)(S)-SH	sulfonotrithioic acid

5. Sulfonimidic acids-S(O)(=NH)-OHsulfonimidic acidSulfonimidoperoxoic acids-S(O)(=NH)-OOHsulfonimidoperoxoic acid

Sulfonimidoperoxoic acids modified by replacement with S, Se and/or Te

-S(O)(=NH)-SOH	sulfonimido(thioperoxoic) SO-acid
-S(O)(=NH)-OSH	sulfonimido(thioperoxoic) OS-acid

Sulfonimidic acids modified by replacement with S, Se and Te

-S(O)(=NH)-SH	sulfonimidothioic S-acid		
adiimidia aaida	S(-NH) OH sulforediimidi	0 00i	

6. Sulfonodiimidic acids-S(=NH)2-OHsulfonodiimidic acidSulfonodiimidoperoxoic acids-S(=NH)2-OOHsulfonodiimidoperoxoic acid

Sulfonodiimidoperoxoic acids modified by replacement with S, Se and/or Te

-S(=NH) ₂ -SOH	sulfonodiimido(thioperoxoic) SO-acid
-S(=NH) ₂ -OSH	sulfonodiimido(thioperoxoic) OS-acid
Sulfonodiimidic acids modified	by replacement with S, Se and/or Te

-S(=NH)₂-SeH sulfonodiimidoselenoic acid

7. Sulfonohydrazonic acids $-S(O)(=NNH_2)-OH$ sulfonohydrazonic acid

Sulfonohydrazonoperoxoic acids -S(O)=(NNH₂)-OOH sulfonohydrazonoperoxoic acid Sulfonohydrazonoperoxoic acids modified by replacement with S, Se and/or Te

-S(S)(=NNH₂)-OOH sulfonohydrazonoperoxothioic acid

Sulfonohydrazonic acids modified by replacement with S, Se and/or Te

$-S(S)(=NNH_2)-OH$	sulfonohydrazonothioic O-acid
-S(O)(=NNH ₂ -SH	sulfonohydrazonothioic S-acid

8. Sulfonodihydrazonic acids $-S(=NNH_2)_2OH$ sulfonodihydrazonic acid Sulfonodihydrazonoperoxoic acids $-S(=NNH_2)_2-OOH$ sulfonodihydrazonoperoxoic acid

Sulfonodihydrazonoperoxoic acids modified by replacement by S, Se and/or Te

-S(=NNH₂)₂-SOH sulfonodihydrazono(thioperoxoic) *O*-acid

Sulfonodihydrazonic acids modified replacement with S, Se and/or Te			
-S(=NI	NH ₂) ₂ -SH	sulfonodihydrazonothioic acid	
9. Sulfinic acids	-SO-OH	H sulfinic acid	
Sulfinoperoxoic acid	-SO-OC	OH sulfinoperoxoic acid	
Sulfinoperoxoi	c acid modified	by replacement with S, Se and/or Te	
-S(O)(S)-OOH	sulfinoperoxothioic acid	
-SO-S0	ЭН	sulfino(thioperoxoic) SO-acid	
-SO-O	SH	sulfino(thioperoxoic) OS-acid	
Sulfinic acids modifi	ed by replacemen	t with S, Se and/or Te	
-SS-Ol	Η	sulfinothioic O-acid	
-SO-Se	eΗ	sulfinoselenoic Se-acid	
10. Sulfinimidic acids	_	S(=NH)-OH sulfinimidic acid	
Sulfinoimidoperoxo	ic acids	-S(=NH)-OOH sulfinimidoperoxoic acid	
Sulfinoimidope	roxoic acids mod	ified by replacement with S, Se and/or Te	
-S(=NH)-OSH		sulfinimido(thioperoxoic) S-acid	
Sulfinimidic	acids modified by	y replacement with S, Se and/or Te	
-S(=NI	H)-SH	sulfinimidothioic acid	
11. Sulfinohydrazonic a	icids –	S(=NNH ₂)-OH sulfinohydrazonic acid	
		-S(=NNH ₂)-OOH sulfinohydrazonoperoxoic acid	
Sulfinohydrazo	noperoxoic acids	modified by replacement with S, Se and/or Te	
-	NH ₂)-SSeH	sulfinohydrazono(selenothioperoxoic) Se-acid	
Sulfinohydrazonic a	cids modified by	replacement with S, Se and/or Te	
	NH ₂)-TeH	sulfinohydrazonotelluroic acid	
12. Selenonic acids	-SeO ₂ -OH	selenonic acid (as for sulfonic acids)	
13. Seleninic acids	-SeO-OH	seleninic acid (as for sulfinic acids)	
14. Telluronic acids	-TeO ₂ -OH	telluronic acid (as for sulfonic acids)	
15. Tellurinic acids	-ТеО-ОН	tellurinic acid (as for sulfinic acids)	
16. Carboxamides	-CO-NH ₂	carboxamide	

-((C)O-NH ₂	amide	
Carboxamides modified by replacement		with S, Se and/or Te	
CS-NH ₂ (C)S-NH ₂		carbothioamide thioamide	
17. Carboximidamides	-C(=NH)-NH ₂ -(C)(=NH)-NH ₂	carboximidamide imidamide	
18. Carbohydrazonamides	-C(=NNH ₂)-NH ₂ -(C)(=NNH ₂)-N	carbohydrazonamide NH ₂ hydrazonamide	
19. Sulfonamides	-SO ₂ -NH ₂ su	fonamide	
Sulfonamides modifi	ed by replacement w	vith S, Se and/or Te	
-S(O)(S)-NF	H ₂ sulfonot	hioamide	
-S(S)(Se)-N	H ₂ sulfonos	elenothioamide	
20. Sulfonimidamides	-S(O)(=NH)-NH ₂	sulfonimidamide	
Sulfonimidamides modifie	ed by replacement v	vith S, Se and/or Te	
-S(S)(=NH)	-NH ₂	sulfonimidothioamide	
21. Sulfonodiimidamides	-S(=NH)2-N	H ₂ sulfonodiimidamide	
22. Sulfonohydrazonamides	-S(O)(=NNF	1 ₂)-NH ₂ sulfonohydrazonamide	
Sulfonohydrazonamides modified by replacement with S, Se and/or Te			
-S(S)(=NH)	-NH ₂	sulfonohydrazonothioamide	
23. Sulfonodihydrazonamide	s –S(=NNH ₂	₂ -NH ₂ sulfonodihydrazonamide	
24. Sulfinamides –SC	0-NH ₂ sulfi	namide	
Sulfinamides modifie	ed by replacement v	vith S, Se and/or Te	
-S(Se)-NH ₂	sulfinos	elenoamide	
25. Sulfinimidamides	-S(=NH)-NH ₂	sulfinimidamide	
26. Sulfinohydrazonamides	-S(=NNH ₂)-NH	2 sulfinohydrazonamide	
27. Selenonamides28. Seleninamides29. Telluronamides30. Tellurinamides	-SeO ₂ -NH ₂ -SeO-NH ₂ -TeO ₂ -NH ₂ -TeO-NH ₂	selenonamide (as for sulfonamides) seleninamide (as for sulfinamides) telluronamide (as for sulfonamides) tellurinamide (as for sulfinamide)	

31. Carbohydrazides $-CO-NHNH_2$ carbohydrazide $-(C)O-NHNH_2$ hydrazide
Carbohydrazides modified by replacement with S, Se and/orTe
-CS-NHNH ₂ carbothiohydrazide
32. Carboximidohydrazides $-C(=NH)-NHNH_2$ carboximidohydrazide imidohydrazide imidohydrazide
33. Carbohydrazonohydrazides $-C(=NNH_2)-NHNH_2$ carbohydrazonohydrazide $-(C)(=NNH_2)-NHNH_2$ hydrazonohydrazide
34. Sulfonohydrazides –SO ₂ -NHNH ₂ sulfonohydrazide
Sulfonohydrazides modified by replacement with S, Se and/or Te
-S(O)(S)-NHNH ₂ sulfonothiohydrazide
35. Sulfonimidohydrazides $-S(O)(=NH)-NHNH_2$ sulfonimidohydrazide
Sulfonimidohydrazides modified by replacement with S, Se and/or Te
$-S(Se)(=NH)-NHNH_2$ sulfonimidoselenohydrazide
36. Sulfonodiimidohydrazides $-S(=NH)_2-NHNH_2$ sulfonodiimidohydrazide
37. Sulfonohydrazonohydrazides $-S(O)(=NNH_2)-NHNH_2$ sulfonohydrazonohydrazide
Sulfonohydrazonohydrazides modified by replacement with S, Se andor Te
-S(Te)(=NNH ₂)-NHNH ₂ sulfonohydrazonotellurohydrazide
38. Sulfonodihydrazonohydrazides $-S(=NNH_2)_2-NHNH_2$ sulfonodihydrazonohydrazide
39. Sulfinohydrazides $-S(O)$ -NHNH ₂ sulfinohydrazide
Sulfinohydrazides modified by replacement with S, Se and/or Te
$-S(Se)-NHNH_2$ sulfinoselenohydrazide
40. Sulfinimidohydrazides $-S(=NH)-NHNH_2$ sulfinimidohydrazide
41. Sulfinohydrazonohydrazides $-S(=NNH_2)-NHNH_2$ sulfinodihydrazonohydrazides
42. Selenonohydrazides $-SeO_2$ -NHNH ₂ selenonohydrazide (as for sulfonohydrazides)
43. Seleninohydrazides $-Se(O)-NHNH_2$ seleninohydrazides (as for sulfinohydrazides)
44. Telluronohydrazides $-\text{TeO}_2$ -NHNH ₂ telluronohydrazides (as for sulfonohydrazides)
45 . Tellurinohydrazides $-Te(O)$ -NHNH ₂ tellurinohydrazides (as for sulfinohydrazides)

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Preferred IUPAC Names Chapter 4, September, 2004

46. Nitriles	-CN -(C)N	carbonitrile nitrile
47. Aldehydes	–СНО –(С)НО	carbaldehyde al
Aldehyd	es modified by replac	ement with S, Se and/or Te
	-CHS -(C)HS	carbothialdehyde thial
	-CHSe -(C)HSe	carboselenaldehyde selenal
	-СНТе -(С)НТе	carbotelluraldehyde tellural
48. Ketones, pse	udoketones, and hete	rones >(C)=O one
Ketones	, pseudoketones, and	heterones modified by replacement with S, Se and/or Te
2	>(C)=S	thione
2	>(C)=Se	selone (not selenone)
	>(C)=Te	tellone (not tellurone)
49. Hydroxy con	npounds	–OH ol
Hydroxy	compounds modified	d by replacement with S, Se and/or Te
-	-SeH selen	ol
-	-TeH tellur	ol
50. Hydroperoxi	des –OOI	H peroxol
Hydrop	eroxides modified by	replacement with S, Se and/or Te
-	–OSH OS-th	nioperoxol
	-SOH SO-th	nioperoxol (not sulfenic acid)
51. Amines	$-NH_2$	amine
52. Imines	=NH	imine
SE		

P-44 Seniority order of parent structures

P-44.0 IntroductionP-44.1 Seniority order of parent structuresP-44.2 Seniority of rings and ring systemsP-44.3 Seniority of chains (the principal chain)P-44.4 Criteria applicable to both rings and chains

P-44.0 Introduction

The selection of parent hydrides is based on the seniority of classes (see P-41), giving priority to suffixes. This order of seniority is also used to choose a parent hydride when different classes are present and between rings and chains. Section P-44.1 covers the selection of parent hydrides when different classes are involved and between rings and chains in the same class. When there is a choice among cyclic parent hydrides, the senior ring or ring system is chosen in accord with the seniority order of rings and ring systems (see P-44.2). When there is a choice among acyclic parent hydrides a principal chain must be chosen (see P-44.3). The three seniority orders, for classes, rings and ring systems, and the principal chain, are expressed in a general seniority order called 'seniority order of parent structures'. Section P-44.4 covers more criteria applicable to both rings and chains.

A thorough revision and extension of the seniority order of classes, of rings and ring systems, and for selecting the principal chain was needed in the context of preferred names.

This revision leads to a major change. In this document, it is recommended to invert the traditional order of seniority between unsaturation and length in the case of acyclic compounds; thus, the first criterion is concerned with the length of the chain and unsaturation is second to length.

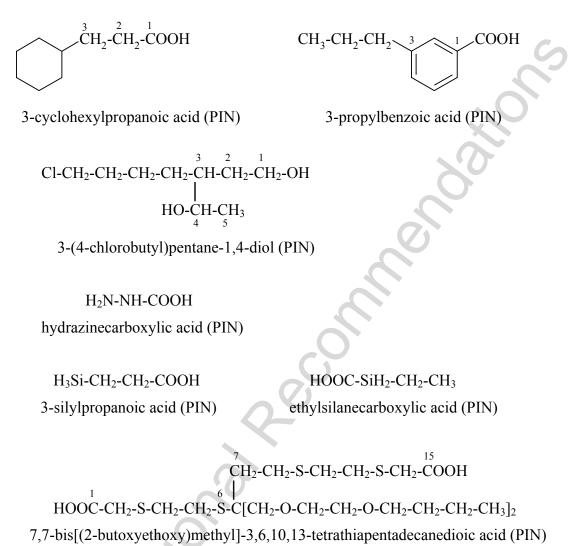
P-44.1 Seniority order of parent structures

When there is a choice, the senior parent structure is chosen by applying the following criteria, in order, until a decision is reached. These criteria must always be applied before those applicable to rings and ring systems (see P-44.2 and P-44.4) and to chains (see P-44.3 and P-44.4).

P-44.1.1 The senior parent structure has the maximum number of substituents corresponding to the principal characteristic group (suffixes) in accord with the seniority of classes (P-41) and the seniority of suffixes (P-43).

Suffixes are used to designate the principal function when attached to chains, rings or ring systems and to any atom, carbon atom or heteroatom.

Examples:



P-44.1.2 The senior parent structure, whether cyclic or acyclic, has the senior atom in accordance with the seniority of classes (see P-41) expressed by the following decreasing element order: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C. This criterion is applied to select the senior atom in chains and to choose between rings and chains. It is not used to choose between rings (see P-44.2) or to select the principal chain modified by skeletal replacement ('a') nomenclature (see P-15.4).

P-44.1.2.1 When two or more atoms denoting different classes are present in a compound directly bonded to each other, and when the choice for parent compound is between these atoms, the parent compound is the one belonging to the class cited first in the seniority of classes given above. A single senior atom is sufficient to give seniority to the parent hydride.

Examples:

Si(CH₃)₄ tetramethylsilane (PIN)

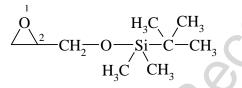
Al(CH₂-CH₃)₃ triethylalumane (PIN) CH₃-PH-SiH₃ methyl(silyl)phosphane (PIN) HS-S-S-S-S-SiH₂-SiH₂-SiH₃ 1-pentasulfanyltrisilane (preselected name)

H₃Si-SiH₂-CH₂-CH₂-PH₃ (2-disilanylethyl)phosphane (PIN) H₃Sb-CH₂-AsH₃ (stibanylmethyl)arsane (PIN)

$$CH_3-CH_2-O-[CH_2-CH_2-O]_3-CH_2-3$$
 SiH₃

3-[(2,5,8,11-tetraoxatridecan-1-yl)cyclohexyl]silane (PIN) (among classes, Si is senior to O, and both are senior to C)

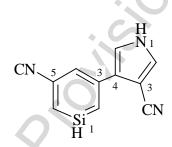
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tert-butyldimethyl(oxiran-2-ylmethoxy)silane (PIN)

HOOC-SiH₂-SiH₂-CH₂-CH₂-COOH

2-(2-carboxyethyl)disilane-1-carboxylic acid (PIN)



4-(5-cyanosilin-3-yl)pyrrole-3-carbonitrile (PIN)

P-44.1.2.2 Systems composed of rings and chains

Two methods are recognized to name systems composed of rings and chains

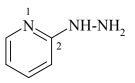
Method (a). Within the same class, a ring or ring system has seniority over a chain. When a ring and a chain contain the same senior element, the ring is chosen as parent. Rings and chains are chosen regardless of their degree of hydrogenation. As a consequence, this approach prefers the choice of a ring over a chain in systems composed of cyclic and acyclic hydrocarbons.

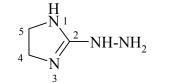
Method (b) The context may favor the ring or the chain, so that, for example, substituents may be treated alike or an unsaturated acyclic structure may be recognized, or the one chosen has the greater number of skeletal atoms in the ring or in the principal chain of the acyclic structure.

In the examples that follow, when a choice is possible, names formed by both methods are given; for preferred IUPAC names method (a) is the choice (see also Chapter 5). Examples:

CH=CH

CH₂-CH₂-CH₂-CH₂-CH₂-CH₂-CH₃ (a) heptylbenzene (PIN) (a) vinylcyclohexane (PIN) (ring preferred to chain) (ring preferred to chain) (b) 1-phenylheptane (b) cyclohexylethene (chain has greater number of (emphasizes unsaturation) skeletal atoms) $^{1}_{\text{CH}=\text{CH}}^{2}$ CH (a) 1,1'-methylenedibenzene (PIN) (a) ethene-1,2-divldicyclohexane (PIN) (ring preferred to chain (ring preferred to chain) as preferred parent) (b) 1,2-dicyclohexylethene (emphasizes unsaturation) (b) diphenylmethane (treats phenyl groups alike as substituents) PH, 1-benzofuran-2-ylphosphane (PIN) 1-(trimethylsilyl)-1H-imidazole (PIN) (P preferred to O) (N preferred to Si)





(a) 2-hydrazinylpyridine (PIN)
 (a) 2-hydrazino-4,5-dihydro-1*H*-imidazole (PIN)
 (ring preferred to chain)

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P-44.1.3 Senior ring or ring system. Criteria that apply only when the choice for parent structure is between two or more rings are given in P-44.2.

P-44.1.4 The principal chain. Criteria that apply only when the choice for parent structure is between two or more chains are given in P-44.3

P-44.1.5 Identical parent structures may differ only in the presence of skeletal atoms with different bonding orders, isotopic modification, or stereochemical configuration. The criteria for such a choice, applicable to either chains or rings, are given in P-44.4.

P-44.2 Seniority order of rings and ring systems

- P-44.2.1 Criteria general to all rings (structural features)
- P-44.2.2 Criteria specific to a particular kind of ring or ring system
- P-44.2.3 Criteria general to all rings (degree of hydrogenation and locants of indicated hydrogen)

P-44.2.1 General criteria for determining ring seniority given below are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior ring or ring system:

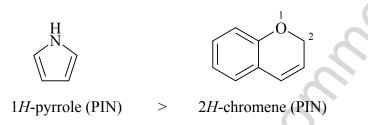
- (a) is a heterocycle;
- (b) has at least one nitrogen atom;
- (c) has at least one heteroatom (in the absence of nitrogen) that occurs earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
- (d) has the greater number of rings;
- (e) has the greater number of ring atoms;
- (f) has the greater number of heteroatoms of any kind;
- (g) has the greater number of heteroatoms occurring earlier in the sequence listed in (c), above.

Each of these criteria is illustrated below.

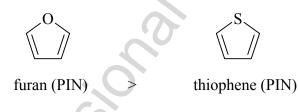
(a) The senior ring or ring system is a heterocycle.

Example: quinoline (PIN) > anthracene (PIN)

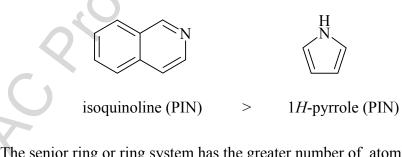
(b) The senior ring or ring system has at least one nitrogen ring atom. Example:



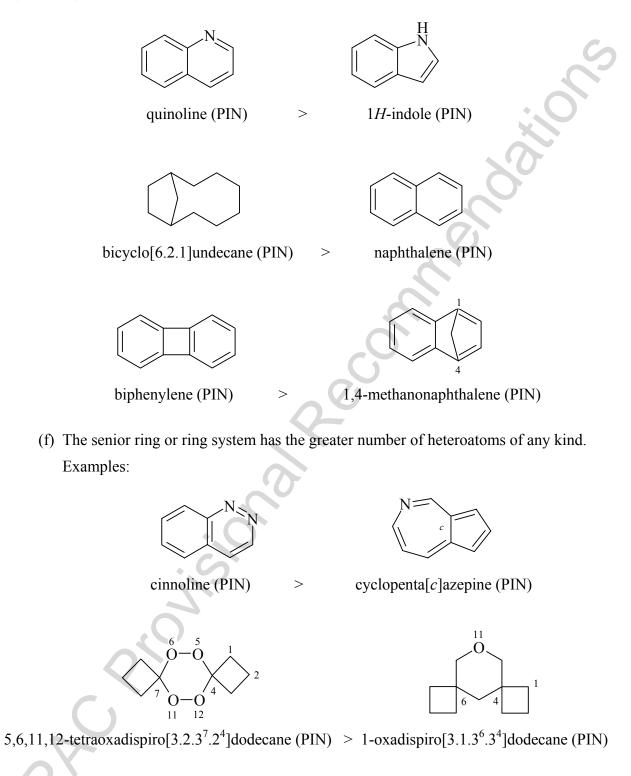
(c) The senior ring or ring system has at least one heteroatom (in the absence of nitrogen) that occurs earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl Example:

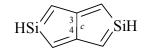


- (d) The senior ring or ring system has the greater number of rings.
 - Example:

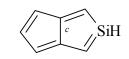


(e) The senior ring or ring system has the greater number of atoms.Examples:

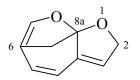


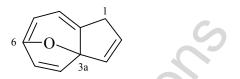


2*H*,5*H*-silolo[3,4-*c*]silole (PIN)

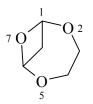


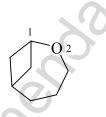
2*H*-cyclopenta[*c*]silole (PIN)





2H-6,8a-methanofuro[2,3-b]oxepine (PIN) > 1H-3a,6-epoxyazulene (PIN)

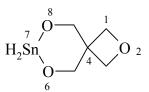


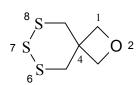


2,5,7-trioxabicyclo[4.1.1]octane (PIN) > 2-oxabicyclo[4.1.1]octane (PIN)

(g) The senior ring or ring system has the greater number of heteroatoms that occur earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:



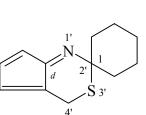


2-oxa-6,7,8-trithiaspiro[3.5]nonane (PIN)

2,6,8-trioxa-7-stannaspiro[3.5]nonane (PIN)

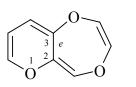
>

>



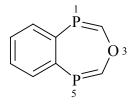
spiro[3,1-benzoxazine-4,1'cyclopentane] (PIN)

O 3

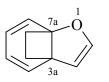


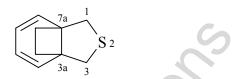
pyrano[3,2-*e*]-1,4-dioxepine (PIN)

4'*H*-spiro[cyclohexane-1,2'-cyclopenta[*d*][1,3]thiazine] (PIN)



3,1,5-benzoxadiphosphepine (PIN)

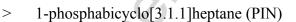




3a,7a-ethano-1-benzofuran (PIN) >



2-oxabicyclo[3.1.1]heptane (PIN)



1H,3H-3a,7a-ethano-2-benzothiophene (PIN)

P-44.2.2 Senority criteria for determining ring seniority applicable to particular types of ring or ring system.

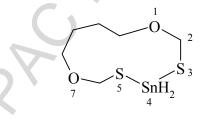
27

- (1) Monocycles (see P-22)
- (2) Polycyclic systems. The senior ring system occurring first in the following list of ring system types.
 - (a) a spiro ring system (see P-23);
 - (b) a cyclic phane system (see P-26);
 - (c) a fused ring system (see P-25);
 - (d) a bridged fused ring system (see P-25);
 - (e) a nonfused bridged ring system (see P-24);
 - (f) an acyclic (linear) phane system (see P-26);
 - (g) a ring assembly (see P-28).

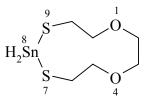
P-44.2.2.1 Senority criteria for determining ring seniority of monocycles.

The senior monocycle:

- (a) has the lower locants for the heteroatoms compared as a set without regard to kind;
 - Example:



1,7-dioxa-3,5-dithia-4-stannacycloundecane (PIN)



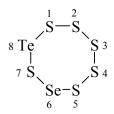
1,4-dioxa-7,9-dithia-8-stannacycloundecane (PIN)

(the set of locants 1,3,4,5,7 is lower than 1,4,7,8,9)

(b) has the lower locants for heteroatoms occuring earlier in the following sequence: F >Cl > Br > I > O > S > Se >Te > N > P > As > Sb > Bi > Si >Sn > Pb > B > Al > Ga > In > Tl.

28

Example:





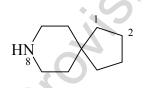
1,2,3,4,5,7,6,8-hexathiaselena->tellurocane (preselected name, see P-12.2)

1,2,3,4,6,7,5,8-hexathiaselenatellurocane (preselected name, see P-12.2)

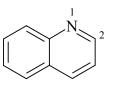
P-44.2.2.2 The senior ring system occurs earliest in the following listing:

- (a) a spiro ring system (see P-44.2.2.2.1);
- (b) a cyclic phane system (see P-44.2.2.2.2);
- (c) a fused ring system (see P-44-2.2.2.3);
- (d) a bridged fused ring system see(P-44.2.2.2.4);
- (e) a nonfused bridged ring system (see P-44.2.2.5);
- (f) an acyclic (linear) phane system (see P-44.2.2.2.6);
- (g) a ring assembly (see P-44.2.2.2.7).

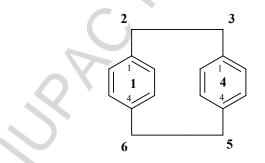
Examples:



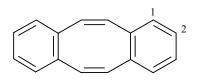
8-azaspiro[4.5]decane (PIN)



quinoline (PIN)

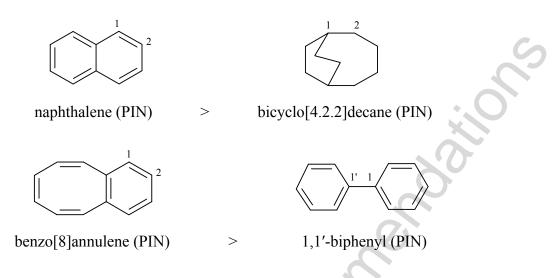


1,4(1,4)-dibenzenacyclohexaphane (PIN)



dibenzo[*a*,*e*][8]annulene (PIN)

>



P-44.2.2.2.1 Senority criteria for spiro ring systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

29

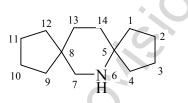
The senior spiro system:

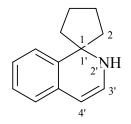
- (a) has the greater number of spiro fusions;
- (b) consists of saturated rings;
- (c) consists of only discrete components.

Each of these criteria is illustrated below.

(a) The senior spiro system has the greater number of spiro fusions.

Example:

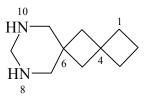


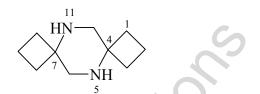


6-azadispiro[$4.2.4^{8}.2^{5}$]tetradecane (PIN) > 2'H-spiro[cyclopentane-1,1'-isoquinoline] (PIN)

(b) The senior spiro system consists of only saturated monocyclic rings and:

- (i) has the lower locant(s) for spiro atom(s);
 - Example:

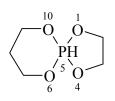




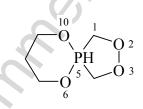
8,10-diazadispiro[$3.1.5^6.1^4$]dodecane (PIN) > 5,11-diazadispiro[$3.2.3^7.2^4$]dodecane (PIN)

(ii) has the lower locants for the heteroatoms compared as a set without regard to kind;

Example:



1,4,6,10-tetraoxa- $5\lambda^5$ -phosphaspiro[4.5]decane (PIN)



2,3,6,10-tetraoxa- $5\lambda^5$ -phosphaspiro[4.5]decane (PIN)

(iii) has the lower locants for heteroatoms that occur earlier in the following sequence; F > Cl > Br > I > O > S > Se > Te > N > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

>

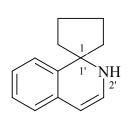
Example:

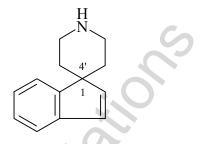


1,7,9-trioxa-2-azaspiro[4.5]decane (PIN) > 3,7,9-trioxa-1-azaspiro[4.5]decane (PIN)

(c) The senior spiro system consists only of discrete components and:

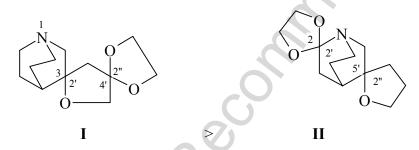
- (i) has the preferred component determined by criteria above and below for the appropriate kind of ring system when the components are compared in their order of seniority;
 - Example:





2'H-spiro[cyclopentane-1,1'-isoquinoline] (PIN) > spiro[indene-1,4'-piperidine] (PIN)

(ii) has the senior component when compared in their order of citation in the name; Example:



- I dispiro[[1]azabicyclo[2.2.2]octane-3,2'-oxolane-4',2"-[1,3]dioxolane] (PIN)
- II dispiro[[1,3]dioxolane-2,2'-[1]azabicyclo[2.2.2]octane-5',2"-oxolane] (PIN)
- (iii) has the lower locants for the spiro atoms in the order of citation in the name.Example:



1'H-spiro[cyclopentane-1,2'-quinoline] (PIN) > 2'H-spiro[cyclopentane-1,3'-quinoline] (PIN)

P-44.2.2.2. Senority criteria for cyclic phane systems given below are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior cyclic phane system:

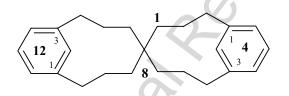
- (a) is the one occurring earlier in the following list of phane skeletal ring systems: spiro, von Baeyer, monocyclic;
- (b) has the senior amplificant, as defined by P-44.2.1.1 through P-44.2.1.7;
- (c) has the lowest superatom locants for all amplificants;

- (d) has the lowest locants for senior amplificants;
- (e) has the lowest attachment locants considered as a set when compared term by term in order of increasing numerical value;
- (f) has the lowest attachment locants when compared term by term in their order of citation in the name;
- (g) has the lowest locants for heteroatoms introduced by skeletal replacement ('a') nomenclature without regard to kind;
- (h) has the lowest locants for heteroatoms introduced by skeletal replacement ('a') nomenclature first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

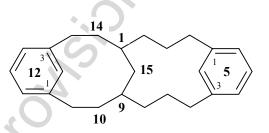
Each of these criteria is illustrated below.

(a) The senior cyclic phane system occurs earlier in the following list of basic phane skeletal ring systems: spiro, von Baeyer, monocyclic.

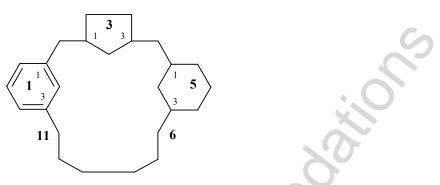
Examples (in order of decreasing seniority according to the above list):



4,12(1,3)-dibenzenaspiro[7.7]pentadecaphane (PIN)

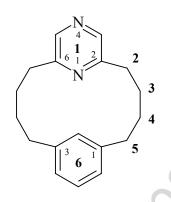


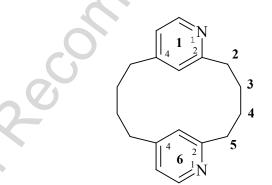
5,12(1,3)-dibenzenabicyclo[7.5.1]pentadecaphane (PIN)



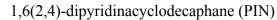
- 1(1,3)-benzena-5(1,3)-cyclohexana-3(1,3)-cyclopentanacycloundecaphane (PIN)
- (b) The senior cyclic phane system has the senior amplificant, as defined by P-44.2.1.1 through P-44.2.1.7.

Example:





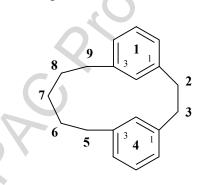
1(2,6)-pyrazina-6(1,3)-benzena->cyclodecaphane (PIN)

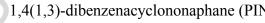


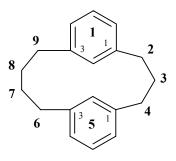
(pyrazine senior to pyridine)

(c) The senior cyclic phane system has the lowest superatom locants for all amplificants.

Example:

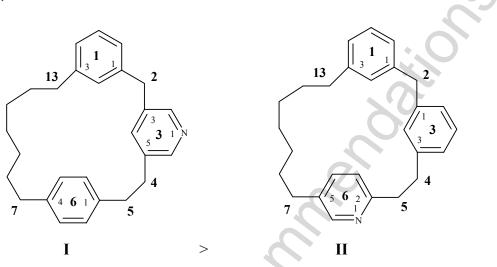






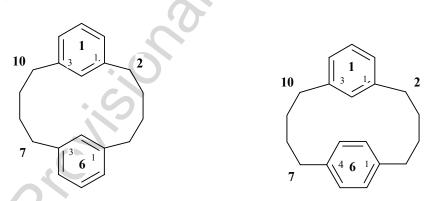
1,4(1,3)-dibenzenacyclononaphane (PIN) > 1,5(1,3)-dibenzenacyclononaphane (PIN)

(d) The senior cyclic phane system has the lowest locants for senior amplificants Example:



- I 3(3,5)-pyridina-1(1,3),6(1,4)-dibenzenacyclotridecaphane (PIN)
 II 6(2,5)-pyridina-1,3(1,3)-dibenzenacyclotridecaphane (PIN)
- 6(2,5)-pyridina-1,3(1,3)-dibenzenacyclotridecaphane (PIN)
- (e) The senior cyclic phane system has the lowest attachment locants considered as a set when compared term by term in order of increasing numerical value.

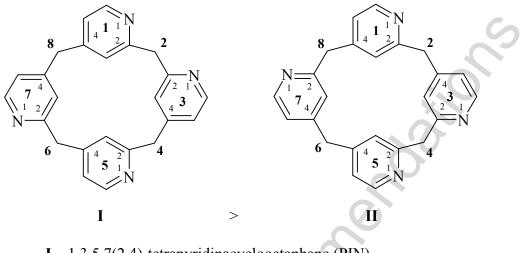
Example:



1,6(1,3)-dibenzenacyclodecaphane (PIN) > 1(1,3),6(1,4)-dibenzenacyclodecaphane (PIN)

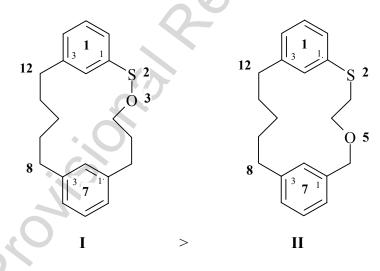
(f) The senior cyclic phane system has the lowest attachment locants when compared term by term in their order of citation in the name.

Example:



- I 1,3,5,7(2,4)-tetrapyridinacyclooctaphane (PIN)
 II 1,5(2,4),3,7(4,2)-tetrapyridinacyclooctaphane (PIN)
- (g) The senior cyclic phane system has the lowest locants for heteroatoms specified by 'a' prefixes without regard to kind

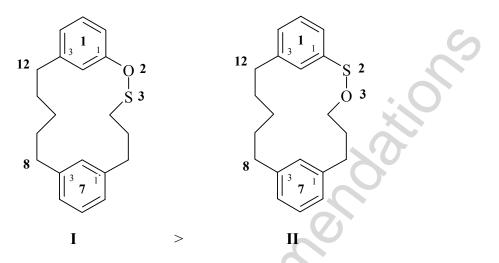
Example:



I 3-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
 II 5-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)

(h) The senior cyclic phane system has the lowest locants for heteroatoms specified by 'a' prefixes first cited in the following order: F > Cl > B > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



I 2-oxa-3-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN) II 3-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)

P-44.2.2.3 Senority criteria for fused ring systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

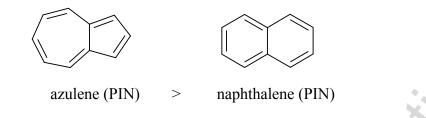
The senior fused ring system:

- (a) has the larger individual ring component at first point of difference when their ring sizes are compared in order of decreasing size;
- (b) has the greater number of rings in a horizontal row (see P-25.3.2.3.2)
- (c) has the lower letters in the expression for ring fusion when compared as a set; letters omitted in names are taken into consideration in the application of this criterion;
- (d) has the lower numbers in the expression for ring fusion, in the order of appearance in a name; locants omitted in names are taken into consideration in application of this criterion;
- (e) has the senior ring system component according to P-44.2.2.5.1 through P-44.2.2.5.4 when its components are compared in order of decreasing seniority;
- (f) has the lower locants for heteroatoms the heteroatoms being compared as a set without regard to kind;
- (g) has the lower locants for heteroatoms occurring earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
- (h) has the lower locants for carbon atoms at fusion sites.

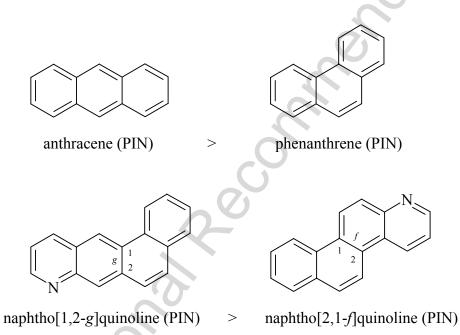
Each of these criteria is illustrated below.

(a) The senior fused ring system has the larger individual ring component at first point of difference when their ring sizes are compared in order of decreasing size.
 Example:

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(b) The senior fused ring system has the greater number of rings in a horizontal row Examples:



(c) The senior fused ring system has the lower letters in the expression for ring fusion when compared as a set; letters omitted in names are taken into consideration in the application of this criterion. [This criterion is valid only for comparing names that have letters; when letters are absent in all names or present in only one name, go to P-44.2.2.4.6 below.]

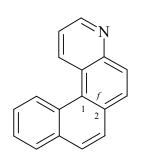
Example:

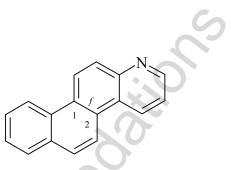


[1,3]dioxolo[c][1,2]oxaphosphole (PIN) > [1,3]dioxolo[d][1,2]oxaphosphole (PIN)

(d) The senior fused ring system has the lower numbers in the expression for ring fusion, in the order of appearance in a name; locants omitted in names are taken into consideration in application of this criterion.

Example:





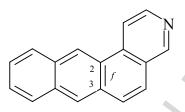
naphtho[1,2-*f*]quinoline (PIN)

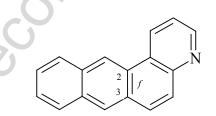
naphtho[2,1-f]quinoline (PIN)

(e) The senior fused ring system has the senior ring system component according to P-44.2.2.4.1 through P-44.2.2.4.4 when its components are compared in order of decreasing seniority

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Example:





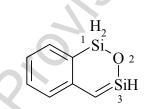
naphtho[2,3-f]quinoline (PIN)

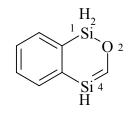
naphtho[2,3-*f*]isoquinoline (PIN)

(f) The senior fused ring system has the lower locants for heteroatoms the heteroatoms being compared as a set without regard to kind.

>

Example:

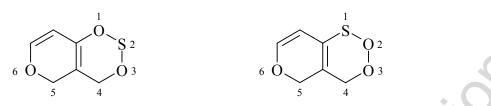




1H-2,1,3-benzoxadisiline (PIN) > 1H-2,1,4-benzoxadisiline (PIN)

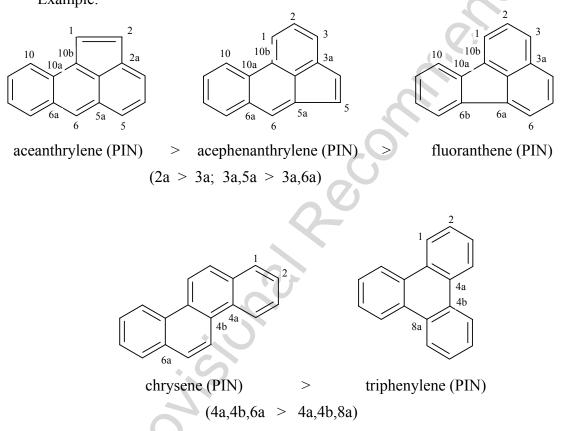
(g) The senior fused ring system has the lower locants for heteroatoms occurring earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



4H, 5H-pyrano[4, 3-d]-1, 3, 2-dioxathiine (PIN) > 4H, 5H-pyrano[4, 3-d]-1, 2, 3-dioxathiine (PIN)

(h) The senior fused ring system has the lowest locants for carbon atoms at fusion sites Example:



P-44.2.2.2.4 Seniority criteria for bridged fused ring systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated. The senior bridged fused ring system:

(a) has the bridged ring system with the greater number of rings before bridging;

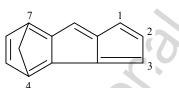
- (b) is the bridged ring system with the greater number of ring atoms before bridging;
- (c) is the bridged ring system with the fewer heteroatoms in the fused ring system;
- (d) is the bridged ring system with the senior fused ring system before bridging according to P-44-2.2.4.1 through P-44.2.2.4.5 and P-44.2.2 above;
- (e) has the lower locants for bridge attachments;

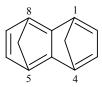
- (f) has the lower locants for heteroatoms in bridges, without regard to kind;
- (g) has the lower locants for heteroatoms in bridges, in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
- (h) has the fewer composite bridges;
- (i) has the fewer dependent bridges;
- (j) has fewer atoms in dependent bridges;
- (k) has the greater number of divalent bridges;
- (1) has lower locants for attachment of independent bridges;
- (m) has the lower locants for attachment of dependent bridges;
- (n) has the fused ring system with the greater number of noncumulative double bonds before bridging.

Each of these criteria is illustrated below.

(a) The senior bridged fused ring system has the bridged ring system with the greater number of rings before bridging.

Example:

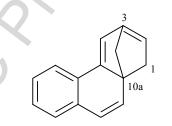


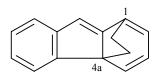


4,7-methanocyclopenta[a]indene (PIN) > 1,4:5,8-dimethanonaphthalene (PIN)

(b) The senior bridged fused ring system is the bridged ring system with the greater number of ring atoms before bridging.

Example:





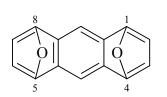
1H-3,10a-methanophenanthrene (PIN)

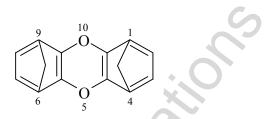
1,4a-ethanofluorene (PIN)

(c) The senior bridged fused ring system is the bridged ring system with the fewer heteroatoms in the fused ring system.

>

Example:





1,4:5,8-diepoxyanthracene (PIN) > 1,4:6,9-dimethanooxanthrene (PIN)

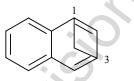
(d) The senior bridged fused ring system is the bridged ring system with the senior fused ring system before bridging according to P-44-2.2.4.1 through P-44.2.2.4.5 and P-44.2.2 above.

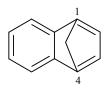
Example:

4,7-methanoazulene (PIN)

1,4-methanonaphthalene (PIN)

(e) The senior bridged ring system has the lowest locants for bridge attachments. Example:

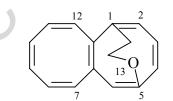


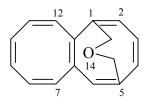


1,3-methanonaphthalene (PIN) > 1,4-methanonaphthalene (PIN)

(f) The senior bridged fused ring system has the lowest locants for heteroatoms in bridges, without regard to kind.

Example:

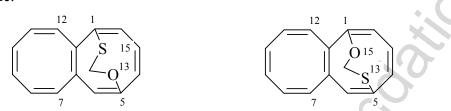




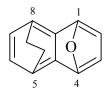
5,1-(epoxyethano)octalene (PIN) > 1,5-(methanooxymethano)octalene (PIN) (locant 13 for the oxygen atom is lower than 14)

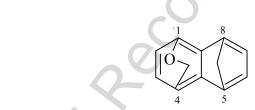
(g) The senior bridged fused ring system has the lowest locants for heteroatoms in bridges, in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. Example:

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- 5,1-(epoxymethanosulfano)octalene (PIN) > 1,5-(epoxymethanosulfano)octalene (PIN) (locant 13 for the oxygen atom is lower than 15)
- (h) The senior bridged fused ring system has the fewer composite bridges. Example:

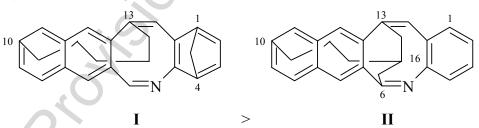




1,4-epoxy-5,8-ethanonaphthalene (PIN) > 1,4-epoxymethano-5,8-methanonaphthalene (PIN)

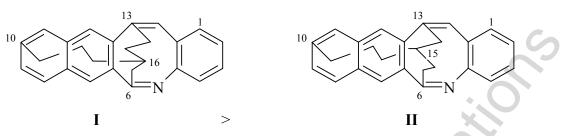
(i) The senior bridged fused ring system has the fewer dependent bridges.

Example:

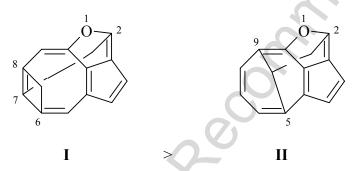


I,4-methano-10,13-pentanonaphtho[2,3-c][1]benzazocine (PIN)
 G,16-methano-10,13-pentanonaphtho[2,3-c][1]benzazocine (PIN)

(j) The senior bridged fused ring system has fewer atoms in dependent bridges.Example:

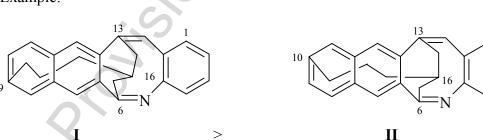


- I 6,16-methano-10,13-hexanonaphtho[2,3-*c*][1]benzazocine (PIN)
- **II** 6,15-ethano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
- (k) The senior bridged fused ring system has the greater number of divalent bridges. Example:



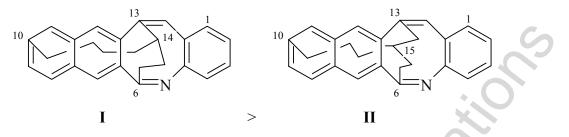
- I 1-oxa-2,7:6,8-dimethanocycloocta[1,2,3-*cd*]pentalene (PIN)
- II 1-oxa-5,9,2-(ethane[1,1,2]triyl)cycloocta[1,2,3-cd]pentalene (PIN)
- (1) The senior bridged fused ring system has lower locants for attachment of independent bridges.

Example:



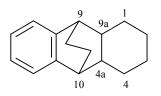
- **I** 6,16-methano-9,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN) **II** 6,16-methano-10,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN)
- (m) The senior bridged fused ring system has the lower locants for attachment of dependent bridges.

Example:



- **I** 6,14-ethano-10,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN) **II** 6,15-ethano-10,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN)
- (n) The senior bridged fused ring system has the fused ring system with the greater number of noncumulative double bonds before bridging.

Example:



1,2,3,4,4a,9,9a,10-octahydro-9,10-ethanoanthracene (PIN)

1,2,3,4,4a,8a,9,9a,10,10a-decahydro-9,10-ethenoanthracene (PIN)

✓ 4a 10

4

P-44.2.2.5 Senority criteria for bridged nonfused ring systems (von Baeyer ring systems) are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior bridged nonfused ring system:

- (a) has the lower number at the first point of difference for describing ring sizes in the descriptor in order of citation;
- (b) has the lower bridge attachment locants (superscript locants) at the first point of difference when compared term by term in order of increasing numerical value;
- (c) has the lower bridge attachment locants (superscript locants) at first point of difference when compared term by term in their order of citation in the name;
- (d) has lowest locants for heteroatoms considered as a set without regard to kind;
- (e) has lowest locants for heteroatoms cited first in the sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Each of these criteria is illustrated below.

(a) The senior bridged nonfused ring system has the lower number at the first point of difference for describing ring sizes in the descriptor in order of citation.



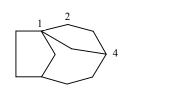
bicyclo[2.2.2]octane (PIN)

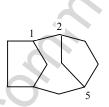
bicyclo[3.2.1]octane (PIN)

(b) The senior bridged nonfused ring system has the lower bridge attachment locants (superscript locants) at the first point of difference when compared term by term in order of increasing numerical value.

>

Example:





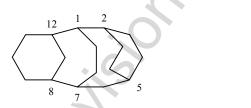
tricyclo[5.2.1.1^{1,4}]undecane (PIN)

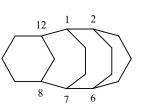
tricyclo[5.2.1.1^{2,5}]undecane (PIN)

(c) The senior bridged nonfused ring system has the lower bridge attachment locants (superscript locants) at first point of difference when compared term by term in their order of citation in the name.

>

Example:

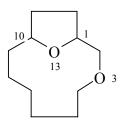


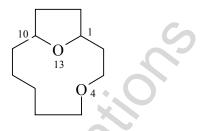


tetracyclo[$5.5.2.2^{2,5}.1^{8,12}$]heptadecane (PIN) > tetracyclo[$5.5.2.2^{2,6}.1^{8,12}$]heptadecane (PIN)

(d) The senior bridged nonfused ring system has lowest locants for heteroatoms considered as a set without regard to kind.

Example:





3,13-dioxabicyclo[8.2.1]tridecane (PIN) > 4,13-dioxabicyclo[8.2.1]tridecane (PIN)

(e) The senior bridged nonfused ring system has lowest locants for heteroatoms cited first in the sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. Example:



2-thia-4,6-diazabicyclo[3.2.0]heptane (PIN) > 4-thia-2,6-diazabicyclo[3.2.0]heptane (PIN)

HN

P-44.2.2.2.6 Senority criteria for acyclic (linear) phane systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated. The senior acyclic (linear) phane system:

- (a) has the senior amplificant, as defined by P-44.2.2.1 through P-44.2.2.5;
- (b) has the lowest set of superatom locants for all amplificants;
- (c) has the lowest locants for senior amplificants;
- (d) has the lowest amplificant attachment locants considered as a set when compared term by term in order of increasing numerical value;
- (e) has the lowest attachment locants when compared term by term in their order of citation in the name;
- (f) has the lowest locants for heteroatoms described 'a' prefixes without regard to kind;
- (g) has the lowest locants for heteroatoms described by 'a' prefixes first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Each of these criteria is illustrated below.

(a) The senior acyclic phane system has the senior amplificant, as defined by P-44.2.2.1 through P-44.2.2.5.

Examples:

6 2 4 CH₂ CH₂ CH₂ 1 1 3 3 3 5 7 **(I)** 4 6 2 CH CH₂ CH-1 3 3 5 7 1 **(II)** (II) 1,7(1),3,5(1,3)-tetrabenzena-(I) 1(3)-pyridina-3,5(1,3),7(1)-> tribenzenaheptaphane (PIN) heptaphane (PIN) [the amplificant pyridine in (I) is senior to the amplificant benzene in (II)] 4 6 2 CH₂ CH₂ CH₂ 7 3 5 **(I)** 4 6 2 CH₂ CH₂ CH, 1 3 3 5 7 1 **(II)** (I) 1(3)-pyridazina-3,5(1,3),7(1)-(II) 1(2)-pyrazina-3,5(1,3),7(1)->

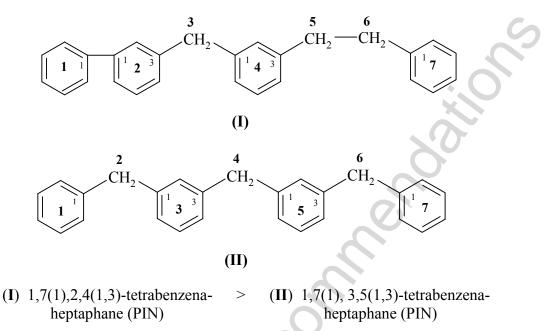
[the amplificant pyridazine in (I) is senior to the amplificant pyrazine in (II)]

tribenzenaheptaphane (PIN)

(b) The senior acyclic phane ring system has the lowest set of superatom locants for all amplificants.

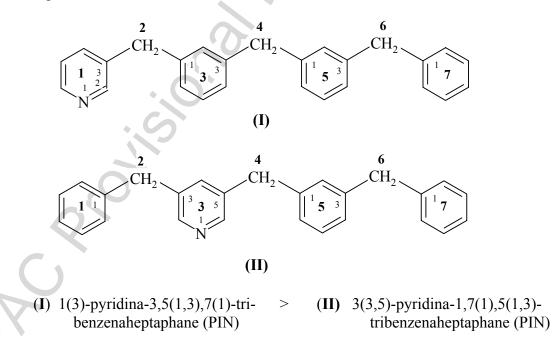
tribenzenaheptaphane (PIN)

Example:



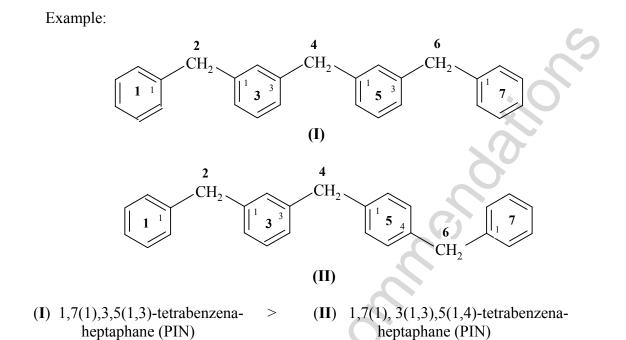
[the locant set '1,2,4,7 ' in (**I**) is lower than '1,3,5,7' in (**II**)]

(c) The senior acyclic phane ring system has the lowest locants for senior amplificants Example:



[the senior amplificant, pyridine, has the lower locant '1' in (I)]

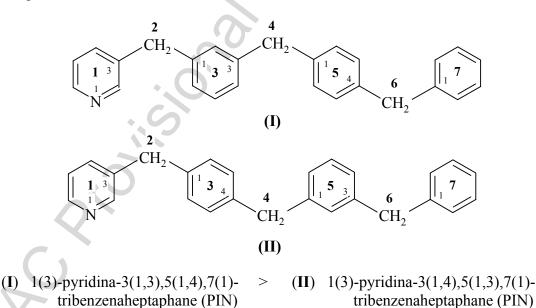
(d) The senior acyclic phane ring system has the lowest amplificant attachment locants considered as a set when compared term by term in order of increasing numerical value.



[the locant set '1,1,1,1,3,3' in (**I**) is lower than '1,1,1,1,3,4' in (**II**)]

(e) The senior phane ring system has the lowest attachment locants when compared term by term in their order of citation in the name.

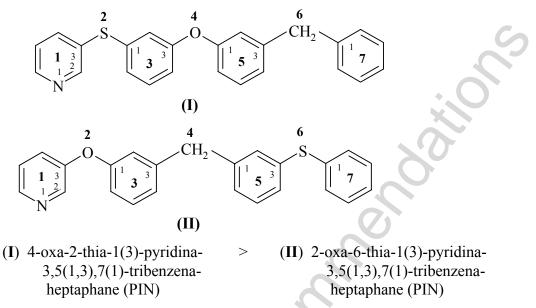
Example:



[the locant set '3,1,3,1,4' in (**I**) is lower than '3,1,4,1,3' in (**II**)]

(f) The senior acyclic phane ring system has the lower locants for heteroatoms described by 'a' prefixes without regard to kind.

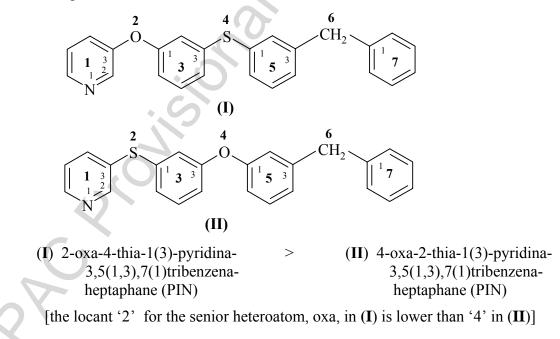
Example:



[the locant set '2,4' for S and O in (I) is lower than '2,6' in (II)]

(g) The senior acyclic phane ring system has the lowest locants for heteroatoms described by ('a') prefixes first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



P-44.2.2.2.7 Senority criteria for ring assemblies are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

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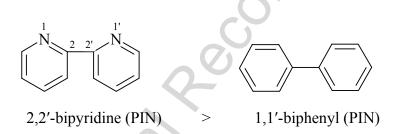
The senior bridged nonfused ring system:

- (a) has the senior component according to the appropriate criteria for rings and ring systems in P-44.2.2.1 through P-44.2.2.6;
- (b) has the lower ring junction locants at the first point of difference when compared term by term in order of increasing numerical value;
- (c) has the lower ring junction locants at the first point of difference when compared term by term in order of their appearance in the name;

Each of these criteria is illustrated below.

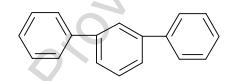
(a) The senior ring assembly has the senior component according to the appropriate criteria for rings and ring systems in P-44.2.2.1 through P-44.2.2.6.

Example:

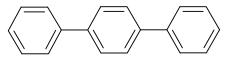


(b) The senior ring assembly has the lower ring junction locants at the first point of difference when compared term by term in order of increasing numerical value. The arabic numbers and letters within parentheses refer to the method of name formation (see P-28.2.1) and the method of numbering (see P-28.3.1)

Example:



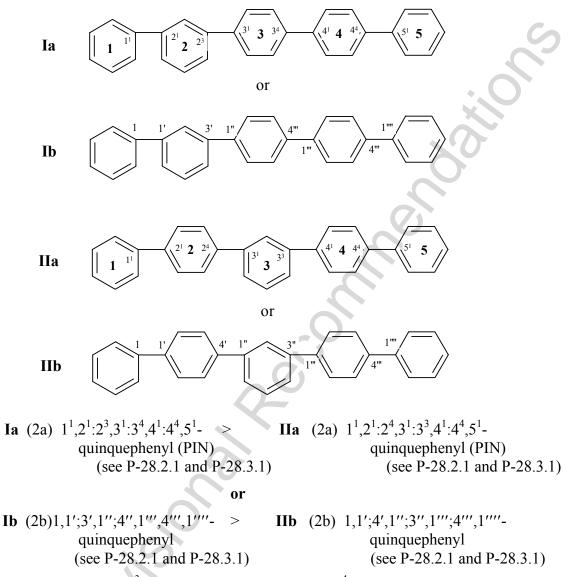
(2a) $1^{1}, 2^{1}: 2^{3}, 3^{1}$ -terphenyl (PIN) (see P-28.2.1 and P-28.3.1) (2b) 1,1':3',1"-terphenyl (see P-28.2.1 and P-28.3.1)



(2a) $1^{1}, 2^{1}: 2^{4}, 3^{1}$ -terphenyl (PIN) >(see P-28.2.1 and P-28.3.1) (2b) 1,1':4',1"-terphenyl (see P-28.2.1 and P-28.3.1)

(c) The senior ring assembly has the lower ring junction locants at the first point of difference when compared term by term in order of their appearance in the name. Example:

>



(at the third term, 2^3 in **Ia** or 3' in **Ib** is lower than 2^4 in **IIb** or 4' in **IIb**)

P-44.2.3 Senority criteria applicable to all rings and ring systems. They are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior ring or ring system:

(a) has the greater number of multiple bonds;

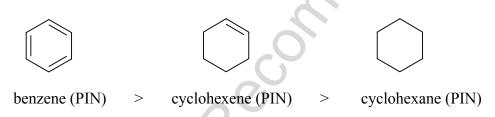
- (b) has the greater number of double bonds;
- (c) has the lower locants for indicated hydrogen;
- (d) has the lower locants for points of attachment (if a substituent group);
- (e) has the lower locant for an attached group expressed as suffix;

- (g) has the maximum number of substituents cited as prefixes;
- (h) has lower locants for substituents named as prefixes;
- (i) has lower locants for the substituent named as a prefix and which is cited first in alphanumerical order.

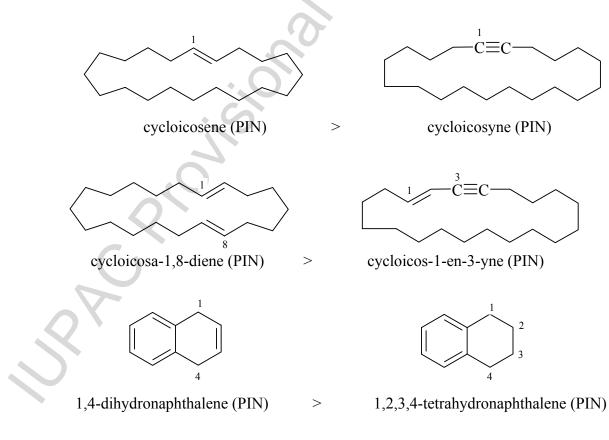
Each of these criteria is illustrated below.

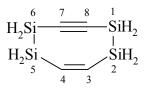
(a) the senior ring or ring system has the greater number of multiple bonds; for the purpose of this criterion, mancude rings or ring systems are considered as consisting of noncumulative double bonds.

Examples:

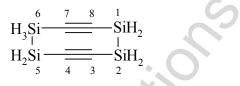


(b) (b) the senior ring or ring system has the greater number of double bonds.





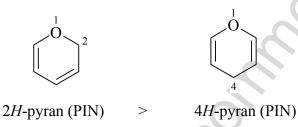
1,2,5,6-tetrasilacyclooct-3-en-7-yne (PIN)



1,2,5,6-tetrasilacycloocta-3,7-diyne (PIN)

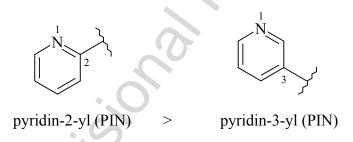
(c) The senior ring or ring system has the lowest locants for indicated hydrogen. Example:

>



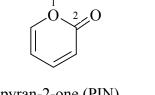
(d) The senior ring or ring system has the lowest locants for points of attachment (if a substituent group).

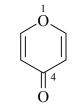
Example:



(e) The senior ring or ring system has the lowest locant for an attached group expressed as suffix.

Example:





2*H*-pyran-2-one (PIN)

4H-pyran-4-one (PIN)

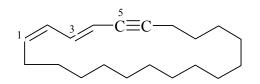
(f) The senior ring or ring system has the lowest locants for endings or prefixes that express changes in the degree of hydrogenation, i.e., for 'ene' and 'yne' endings and 'hydro/dehydro' prefixes.

>

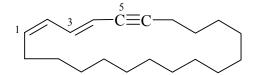
(i) For the endings endings 'ene' and 'yne' lower locants are assigned first to the endings as a set without regard to type and then to 'ene' endings.

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Examples:

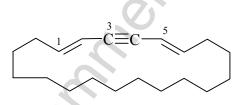


cycloicosa-1,3-dien-5-yne (PIN)



cycloicosa-1,3-dien-5-yne (PIN)

cycloicosa-1,8-dien-3-yne (PIN)



cycloicosa-1,5-dien-3-yne (PIN)

(ii) for 'hydro/dehydro' prefixes, lower locants are assigned as described in P-31.2.4.

>

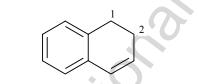
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Examples:



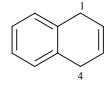
1,2-dihydronaphthalene (PIN)



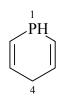
5

1,2-dihydrophosphinine (PIN)

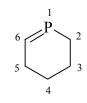
1,2,3,4-tetrahydrophosphinine (PIN)



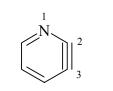
1,4-dihydronaphthalene (PIN)



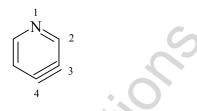
1,4-dihydrophosphinine (PIN)



2,3,4,5-tetrahydrophosphinine (PIN)



2,3-didehydropyridine (PIN)



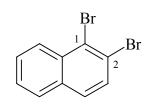
3,4-didehydropyridine (PIN)

(g) The senior ring or ring system has the maximum number of substituents cited as prefixes.

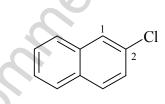
>

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Example:

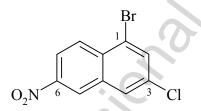


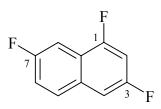
1,2-dibromonaphthalene (PIN)



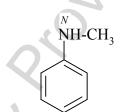
2-chloronaphthalene (PIN)

(h) The senior ring or ring system has lower locants for substituents named as prefixes. Example:

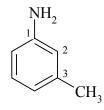




1-bromo-3-chloro-6-nitronaphthalene (PIN) > 1,3,7-trifluoronaphthalene (PIN)

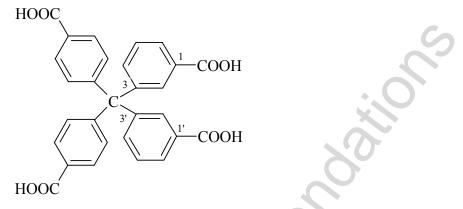


N-methylaniline (PIN)



3-methylaniline (PIN)

>



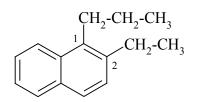
- 3,3'-[bis(4-carboxyphenyl)methylene]dibenzoic acid (PIN) [not 4,4'-[bis(3-carboxyphenyl)methylene]dibenzoic acid; the senior parent structure must be the benzene ring substituted in the 1,3-positions]
- (i) The senior ring or ring system has lower locants for the substituent named as a prefix and which is cited first in alphanumerical order.

>

>

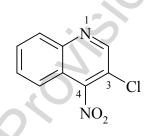
Examples:

CH,-CH, CH₂-CH₂-CH₃

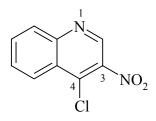


2-ethyl-1-propylnaphthalene (PIN)

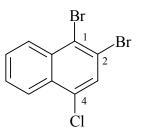
1-ethyl-2-propylnaphthalene (PIN)

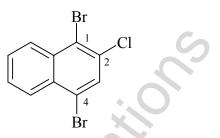


3-chloro-4-nitroquinoline (PIN)



4-chloro-3-nitroquinoline (PIN)







P-44.3 The principal chain

In an acyclic compound, or in a compound composed of chains and rings, the chain on which the nomenclature and numbering is based is called the 'principal chain'. When there is a choice for the principal chain, the following criteria are applied, in the order listed, until a decision is reached.

A change to the traditional order of seniority criteria is recommended; the length of the chain is senior to unsaturation.

The principal chain:

- (a) contains the greater number of heteroatoms;
- (b) has the greater number of skeletal atoms;
- (c) contains the greater number of the most senior acyclic heteroatom in the order: O > OGa > In > Tl;
- (d) has the greater number of double and triple bonds considered together;
- (e) contains the greater number of double bonds;
- (f) has lowest locants for heteroatoms considered together as a set without regard to kind;
- (g) has lowest locants for heteroatoms appearing first in the order: O > S > Se >Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;
- (h) has lowest locants for the principal group (that is for the suffix);
- (i) has lowest locants for multiple bonds;
- (j) has lowest locants for double bonds;

- (k) has the greater number of substituents (other than the principal characteristic group or 'hydro/dehydro') cited as prefixes;
- (1) has the lower locant(s) for all substituents (other than the principal characteristic group or 'hydro/dehydro') cited as detachable prefixes;

(m) has the maximum number of substituents (other than principal characteristic groups or 'hydro/dehydro') cited as prefixes earlier in alphanumerical order.

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Each of these criteria is illustrated below.

(a) The principal chain contains the greater number of acyclic heteroatoms. Examples:

6-(pentyloxy)-2,5,8,11,14-pentaoxahexadecane (PIN) [not 11-(2-methoxyethoxy)-3,6,9,12-tetraoxaheptadecane]

$$CH_3-CH_2-SiH_2-[CH_2-CH_2-SiH_2]_3-CH_2 SiH_3$$

1-(3-silylcyclohexyl)-2,5,8,11-tetrasilatridecane (PIN)

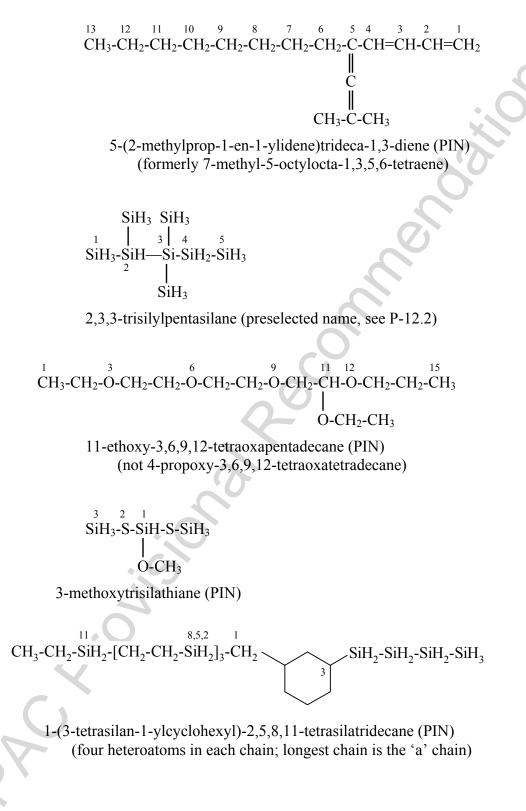
(b) the principal chain has the greater number of skeletal atoms.

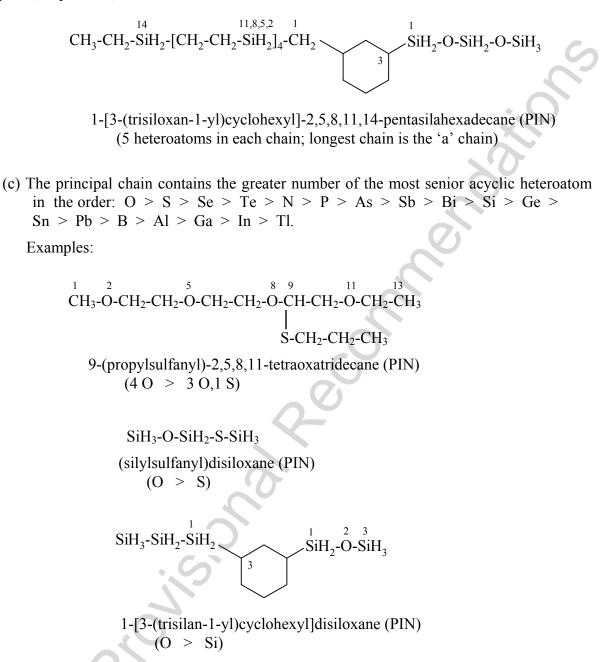
Examples:

$$\begin{array}{c}
5 & 4 & 3 & 2 & 1 \\
CH_3 - CH_2 - CH - CH_2 - CH_3 \\
\downarrow \\
CH_3
\end{array}$$
3-methylpentane (PIN)
(not 2-ethylbutane)
$$\begin{array}{c}
CH_2 \\
8 & 7 & 6 & 5 & 4 \\
CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - CH_3
\end{array}$$

$$\begin{array}{c}
CH_2 \\
8 & 7 & 6 & 5 & 4 \\
CH_3 - CH_2 - CH_2 - CH_2 - CH_2 - CH_3
\end{array}$$

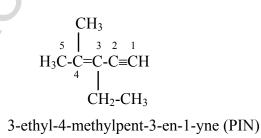
$$\begin{array}{c}
3-methylideneoctane (PIN) \\
(formerly 2-ethylhept-1-ene)
\end{array}$$





(d) The principal chain has the greater number of unsaturated bonds of any kind

Examples:



4-ethoxy-3,6,9,12-tetraoxatetradec-1-ene (PIN)

(e) The principal chain contains the greater number of double bonds. Example:

$$H_{2}C = CH - CH_{2} - CH - CH_{2} -$$

- 4-(prop-1-yn-1-yl)hepta-1,6-diene (PIN)
- (f) The principal chain expresses lowest locants for heteroatoms considered together as a set without regard to kind.

Example:

4-(ethylsulfanyl)-2-oxa-6,9,12-trithiatetradecane (PIN) [not 11-(ethylsulfanyl)-13-oxa-3,6,9-trithiatetradecane; the heteroatom locant set 2,6,9,12 is lower than the locant set 3,6,9,13]

(g) The principal chain expresses lowest locants for heteroatoms appearing first in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > A1 > Ga > In > Tl.

Example:

4-[(methylsulfanyl)methyl]-2-oxa-6,9,12-trithiatetradecane (PIN) (O > S for lower locant) (h) The senior parent chain has the lower locant(s) for the characteristic group expressed as a suffix, i.e., the principal group.

Examples:

$$\begin{array}{c} CH_{3} \\ 5 \\ HO-CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH-CH-CH_{2}-CH_{2}-OH \\ & & & \\ & & & \\ & & & \\ & & & \\ CH_{2}-CH-CH_{2}-CI \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & &$$

8-chloro-5-(4-hydroxybutan-2-yl)octane-1,7-diol (PIN) 8-chloro-5-(3-hydroxy-1-methylpropyl)octane-1,7-diol

7-[(2-hydroxyethyl)silyl]-2,4,6,8-tetrasiladecane-1,9-diol (PIN)

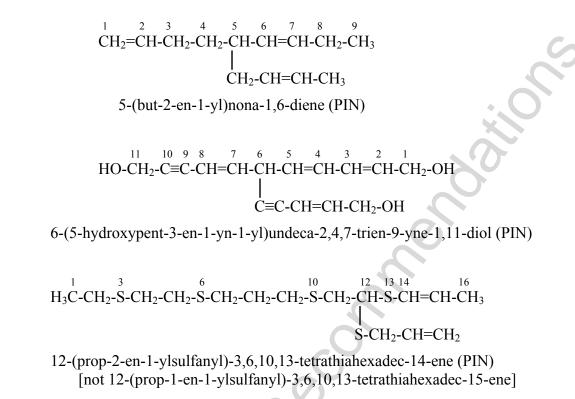
(i) The principal chain has lowest locants for multiple bonds.Examples:

¹¹ ¹⁰ ⁹ ⁸ ⁷ ⁶ ⁵ ⁴ ³ ² ¹

$$CH_3$$
- CH_2 - CH_2 - $C\equiv C$ - CH - CH = CH - CH = CH - CH_3
⁶-(pent-2-yn-1-yl)undeca-2,4-dien-7-yne (PIN)
(the locant set 2,4,7 is lower than 2,4,8)
⁵ ⁶
 CH - CH_3
¹ ² ³ \parallel
 $H_2C=CH$ - C - C - CH = CH_2
 \parallel
 $H_2C=CH$ - C - C - CH = CH_2
 \parallel
 H_2C = CH - CH_3
4-ethenyl-3-ethylidene-1,4-diene (PIN)

(j) The principal chain has the lowest locants for double bonds. Examples:

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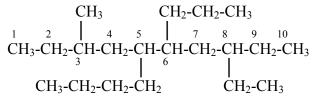


(k) The principal chain has the greater number of substituents (other than the principal characteristic group or 'hydro/dehydro') cited as prefixes.

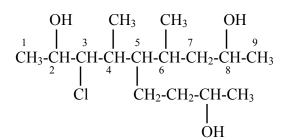
Examples:

 $\begin{array}{c} \begin{array}{c} & 2 & 1 \\ & CH_3-CH-CH_3 \\ & H_3C-CH_2-CH_2-CH-CH_2-CH_3 \\ 3-ethyl-2-methylhexane (PIN) \\ (not 3-isopropylhexane) \\ \end{array}$ $\begin{array}{c} H_3Si \quad SiH_2-SiH_3 \\ 1 & H_3-2iH-SiH_2-SiH_2-SiH_3 \\ 3-disilanyl-2-silylhexasilane (preselected name, see P-12.2) \end{array}$

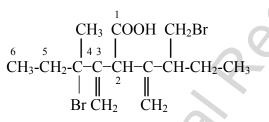
Preferred IUPAC Names Chapter 4, September, 2004



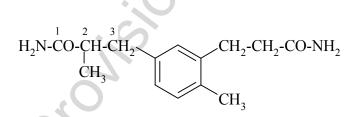
5-butyl-8-ethyl-3-methyl-6-propyldecane (PIN)



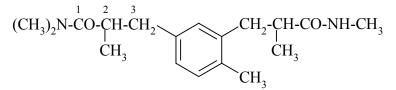
3-chloro-5-(3-hydroxybutyl)-4,6-dimethylnonane-2,8-diol (PIN)



4-bromo-2-[3-(bromomethyl)pent-1-en-2-yl]-4-methyl-3-methylidenehexanoic acid (PIN) 4-bromo-2-[2-(bromomethyl)-1-methylidenebutyl]-4-methyl-3-methylidenehexanoic acid



3-[3-(3-amino-3-oxopropyl)-4-methylphenyl]-2-methylpropanamide (PIN) [not 3-[5-(3-amino-2-methyl-3-oxopropyl)-2-methylphenyl]propanamide; the correct name has 2 substituents; the incorrect name only 1]

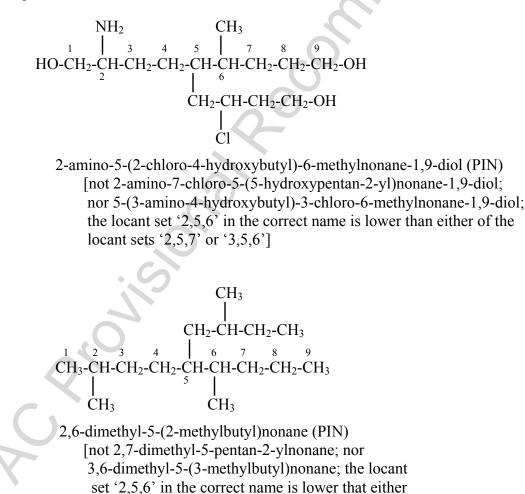


N,*N*,2-trimethyl-3-{4-methyl-3-[2-methyl-3-(methylamino)-3-oxopropyl]phenyl}-propanamide (PIN)

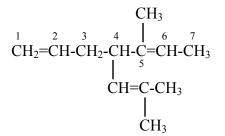
[not 3-{5-[(3-dimethylamino)-2-methyl-3-oxopropyl]-2-methylphenyl}-*N*,2-dimethylpropanamide; the correct name has 4 substituents, the incorrect name has only 3]

(l) The principal chain has the lower locant(s) for substituents (other than the principal characteristic group or 'hydro/dehydro') cited as detachable prefixes.

Examples:



of the locant sets '2,5,7' or '3,5,7']



5-methyl-4-(2-methylprop-1-en-1-yl)hepta-1,5-diene (PIN) [not 4-but-2-en-2-yl-6-methylhepta-1,5-diene; the locant set '4,5' is lower than '4,6']

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- 3-[5-(3-amino-2-methyl-3-oxopropyl)-2-methylphenyl]-*N*-methylpropanamide (PIN) [not 2-methyl-3-{3-[3-(methylamino)-3-oxopropyl]-4-methylphenyl}propanamide; the locant set *N*,3 in the correct name is lower than 2,3 (see P-14.3.4)]
- (m) The principal chain has the maximum number of substituents (other than principal characteristic groups or 'hydro/dehydro') cited as prefixes earlier in alphanumerical order, i.e., when two series of substituent names in alphanumerical order are compared term by term the series that contains the earlier term at the first difference is preferred.

not

Examples:

4-bromo-2-(2-chloroethyl)butan-1-ol (PIN) 2-(2-

Br-CH₂-CH

CH₂-OH

2-(2-bromoethyl)-4-chlorobutan-1-ol

('bromo' precedes 'bromoethyl' in alphanumerical order)

$$\begin{array}{c} & & 6 \\ \text{Br-CH}_2\text{-CH-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CHClBr} \\ & & \text{I} \\ \text{CH}_2\text{-Cl} \end{array} \quad \text{not}$$

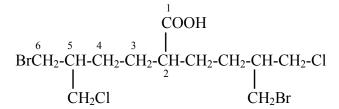
Br-CH₂-CH-CH₂-CH₂-CH₂-CH₂-CHClBr
$$|$$

 CH_2 -Cl

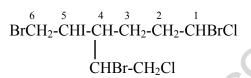
1,6-dibromo-1-chloro-5-(chloromethyl)hexane (PIN) 1-bromo-5-(bromomethyl)-1,6-dichlorohexane

[the correct name has two bromo prefixes viewed as bromo-, bromo-, the incorrect

name has only one bromo prefix; the numerical term is ignored and thus the alphanumerical comparison is 'bromo-,bromo-,chloro' with 'bromo-,bromomethyl']

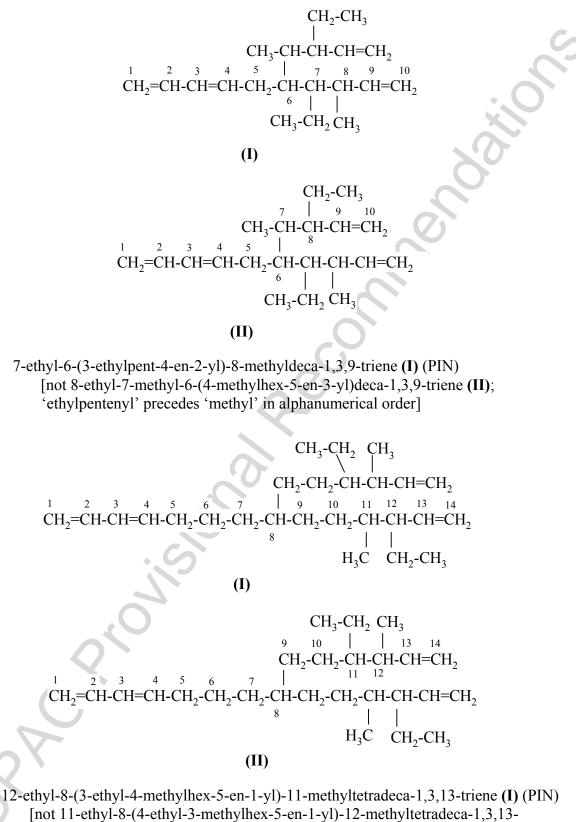


6-bromo-2-[4-bromo-3-(chloromethyl)butyl]-5-(chloromethyl)hexanoic acid (PIN) [not 2-[4-bromo-3-(chloromethyl)butyl]-5-(bromomethyl)-6-chlorohexanoic acid; 'bromo', 'bromo', precedes 'bromo', 'chloromethyl' in alphanumerical order]

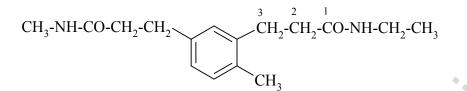


1,6-dibromo-4-(1-bromo-2-chloroethyl)-1-chloro-5-iodohexane (PIN) [not 1,5-dibromo-4-(2-bromo-1-iodoethyl)-1,6-dichlorohexane; since the two prefixes first cited are identical in number and in alphanumerical order, the next prefixes in order are considered and '(bromo...chloroethyl)' precedes '(bromo...iodoethyl)']

4-bromo-2-(1-bromo-2-hydroxyethyl)-3-hydroxybutanoic acid (PIN) [not 3-bromo-2-(2-bromo-1-hydroxyethyl)-4-hydroxybutanoic acid; '(1-bromo-2-hydroxyethyl)' appears earlier in alphanumerical order than '(2-bromo-1-hydroxyethyl)' (see P-14.5).]



triene(**II**); '(3-ethyl-4-methylhex-5-en-1-yl)' must be cited before '(4-ethyl-3ethyl-5-en-1-yl)']



N-ethyl-3-{2-methyl-5-[3-(methylamino)-3-oxopropyl]phenyl}propanamide (PIN) [not 3-{3-[3-(ethylamino)-3-oxopropyl]-4-methylphenyl}-*N*-methylpropanamide; 'ethyl' precedes 'ethylamino' in alphanumerical order]

P-44.4 Further criteria applicable to rings, ring systems, and principal chains

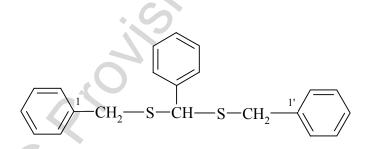
Two or more names may result from using the same parent structures because of multiple occurrences of the parent structure or may differ only in the presence of skeletal atoms with different bonding numbers, isotopic modification, or stereochemical configuration.

- P-44.4.1 Multiplied identical parent structures;
- P-44.4.2 Selection of preferred IUPAC name according to lowest alphanumerical order;
- P-44.4.3 Seniority according to nonstandard bonding numbers;
- P-44.4.4 Senority according to isotopic modification;
- P-44.4.5 Seniority according to configuration.

P-44.4.1 Multiplied identical parent structures

When two or more parent structures, rings, ring systems, or chains, satisfy the requirements for multiplicative nomenclature (see P-15.3), the greater number of parent structures is included as the parent structure by multiplication.

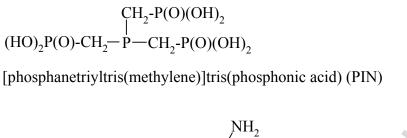
Example:

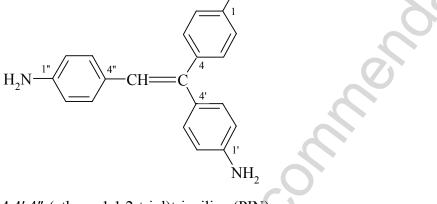


1,1'-[(phenylmethylene)bis(sulfanediylmethylene)]dibenzene (PIN)

HOOC-CH₂ CH₂-COOH HOOC-CH₂-N-CH₂-CH₂-N-CH₂-COOH

N,*N*'-ethane-1,2-diylbis[*N*-(carboxymethyl)glycine] (PIN) 2,2',2",2"'-(ethane-1,2-diyldinitrilo)tetraacetic acid





4,4',4"-(ethene-1,1,2-triyl)trianiline (PIN)

P-44.4.2 Selection of names according to lowest alphanumerical order

When two names can be formed based on the same parent structure, the preferred name is the one that exhibits the lowest alphanumerical order when the names are compared character by character.

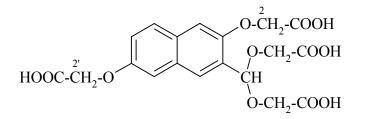
Examples:

CH

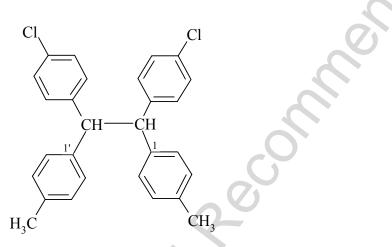
(phenylmethoxy)benzene (PIN) [not (phenoxymethyl)benzene]

CH CH-

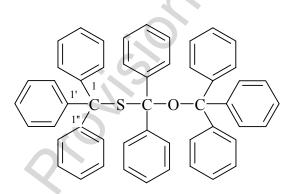
2-[2-(2-oxocyclopentyl)ethylidene]cyclopentan-1-one (PIN) [not 2-[2-(2-oxocyclopentylidene)ethyl]cyclopentan-1-one]



2,2'-({3-[bis(carboxymethoxy)methyl]naphthalene-2,6-diyl}bis(oxy))diacetic acid (PIN) [not 2,2'-({[3,7-bis(carboxymethoxy)naphthalene-2-yl]methanediyl}bis(oxy))diacetic acid]



1,1'-[1,2-bis(4-chlorophenyl)ethane-1,2-diyl]bis(4-methylbenzene) (PIN) [not 1,1'-[1,2-bis(4-methylphenyl)ethane-1,2-diyl]bis(4-chlorobenzene)



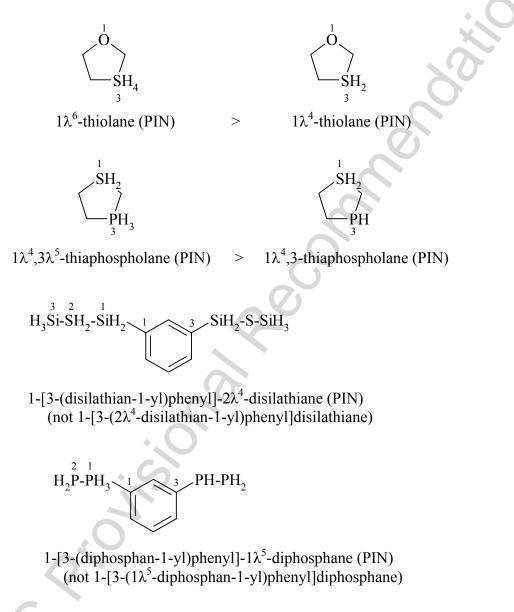
1,1',1"-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methanetriyl)tribenzene (PIN) [not1,1',1"-({diphenyl[(triphenylmethyl)sulfanyl]methoxy}methanetriyl)tribenzene

P-44.4.3 Parent structures in compounds having atoms with nonstandard bonding numbers (see P-14.1)

P-44.4.3.1 When a choice is needed between two chains or two rings or ring systems having skeletal atoms with nonstandard bonding numbers, the one having the maximum number of atoms with nonstandard bonding numbers is chosen as principal chain or senior ring or ring

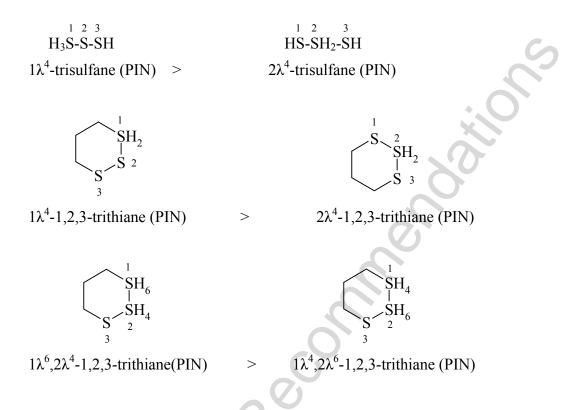
system. If a further choice is needed between the same skeletal atom with two different nonstandard bonding numbers, preference for the senior parent structure is given in order of the decreasing numerical value of the bonding number, i.e., λ^6 is preferred to λ^4 .

Examples:



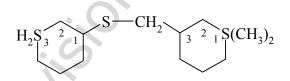
P-44.4.3.2 When a choice is needed between two chains or rings or ring systems having skeletal atoms with nonstandard bonding numbers, the one having the lowest locants for atoms with nonstandard bonding numbers is chosen as principal chain or senior ring or ring system. If a further choice is needed, the atom with the highest bonding number receives the lowest locant.

Examples:

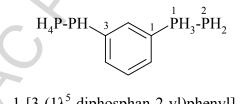


P-44.4.3.3 When a choice between two chains or rings or ring systems having the same skeletal atoms with nonstandard bonding numbers, the parent chain or ring or ring system as that with the greater number of substituents. If a choice still remains, the parent chain or ring or ring system is the one with substituents having the lower locants.

Example:



 $3-\{[(dihydro-1\lambda^4-thiopyran-3(2H)-yl)sulfanyl]methyl\}-1,1-dimethyltetrahydro-1\lambda^4-thiopyran (PIN) (greater number of substituents)$



1-[3-($1\lambda^5$ -diphosphan-2-yl)phenyl]- $1\lambda^5$ -diphosphane (PIN) (not 2-[3-($1\lambda^5$ -diphosphan-1-yl)phenyl]- $1\lambda^5$ -diphosphane; lower locant for substituent)

P-44.4.3.4 When a choice for principal chain is needed between two chains having substituent groups differing only by their bonding numbers, that chain having the greater number of substituent group(s) with the higher bonding number is selected as principal chain. If a further choice is needed, that chain having the lowest locants for atoms with the higher bonding number is selected as principal chain.

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Examples:

$$H_{4}P-CH_{2}-CH-COOH$$

$$H_{2}-PH_{2}$$

 $3-(\lambda^5-phosphanyl)-2-(phosphanylmethyl)propanoic acid (PIN)$

 $4-(1\lambda^5-diphosphan-2-yl)-2-(diphosphan-1-ylethyl)$ butanenitrile (PIN)

$$\begin{array}{c} \begin{array}{c} 3 & 2 & 1 \\ H_6S-CH_2-CH-COOH \\ \\ \\ \\ \\ CH_2-SH_4 \end{array}$$

 $3\lambda^6$ -sulfanyl-2-(λ^4 -sulfanylmethyl)propanoic acid (PIN)

P-44.4.3.5 When a further choice is needed, that chain having the lowest locants for the substituent group(s) with the higher bonding number is selected as principal chain.

Example:

2-(2,3 λ^5 -diphosphanylpropyl)-4 λ^5 ,5-diphosphanylpentanoic acid (PIN)

P-44.4.4 Parent structures with isotopic modification.

When there is a choice for the senior parent structure between isotopically modified and isotopically unmodified compounds (see Chapter 8), the senior parent structure is chosen according to the following criteria, applied successively until a decision can be made. In structures and names, nuclide symbols enclosed in parentheses describe isotopic substitution; nuclide symbols enclosed in square brackets describe isotopic labeling (see Chapter 8).

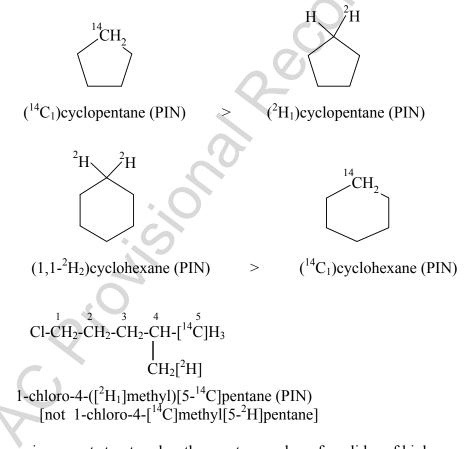
(a) The senior parent structure will contain the greater number of isotopically modified atoms or groups.

Example:

$$\begin{array}{c}1 & 2 & 3 & 4 & 5\\Cl-CH_2-CH_2-CH_2-CH_2-CH-CH_2^2H\\ \\ \\ \\ CH_3\end{array}$$
1-chloro-4-methyl(5-²H₁)pentane (PIN)

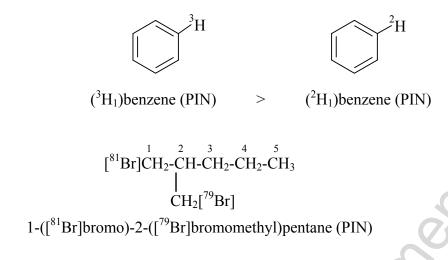
(b) The senior parent structure has the greater number of nuclides of higher atomic number for modified atoms or groups.

Examples:



(c) The senior parent structure has the greater number of nuclides of higher mass number for modified atoms or groups.

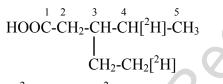
Example:



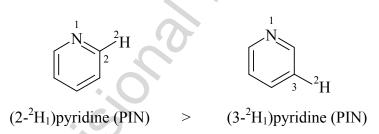
(d) The senior parent structure has the lowest locant(s) for isotopically modified atoms or groups.

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Examples:



3-([2-²H₁]ethyl)[4-²H₁]pentanoic acid (PIN)



(e) The senior parent structure has the lower locant(s) for nuclides of higher atomic number for modified atoms or groups;

Example:

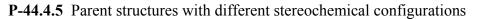
HOOC-CH₂-CH-CH[²H]-[¹³C]H₃
$$[^{13}C]H_2$$
-CH₂[²H]
3-([1-¹³C,2-²H₁]ethyl)[5-¹³C,4-²H₁]pentanoic acid (PIN)

(f) The senior parent structure has the lowest locant(s) for nuclides of higher mass number for modified atoms or groups.

Example:

$$HO-CH_{2}-CH-[^{14}C]H_{2}-[^{13}C]H_{3}$$

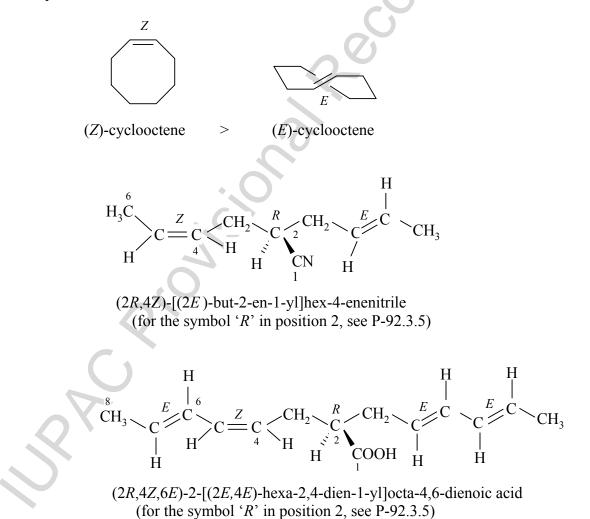
$$[^{13}C]H_{2}-[^{14}C]H_{3}$$
2-([1-¹³C,2-¹⁴C]ethyl)[4-¹³C,3-¹⁴C]butan-1-ol (PIN)

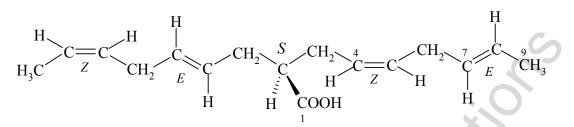


P-44.4.5.1 Choice between '*E*' and '*Z*'

When there is a choice between parent structures that differ only by 'Z' and 'E' configurations, the senior parent structure contains the greater number of double bonds with 'Z' configuration; when a further choice is required, the senior parent structure has the lower locant(s) for the double bond(s) with the 'Z' configuration. For the meaning of 'Z', 'E', 'R', and 'S', see Chapter 9.

Examples:

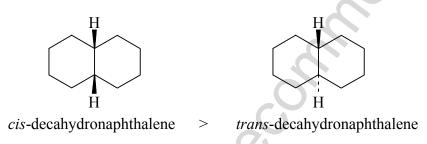




(2*S*,4*Z*,7*E*)-2-[(2*E*,5*Z*)-hepta-2,5-dien-1-yl]nona-4,7-dienoic acid

P-44.4.5.2 In a preferred parent structure, *cis*-configurations are senior to *trans*-configurations.

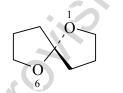
Example:

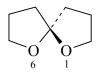


P-44.4.5.3 Choice among chiral centers

When there is a choice between parent structures differing only by the configurations of the chiral centers, the principal chain or the senior ring system is chosen by applying the CIP sequence rules 4 and 5, in the order: *like* stereodescriptors such as 'RR', 'SS' have priority over *unlike* 'RS' and 'SR' ('l' has priority over 'u'), the 'r' over 's', then 'R' over 'S'. The CIP Rules are described in Chapter 9.

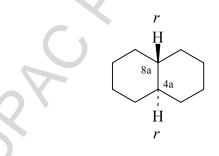
Examples:



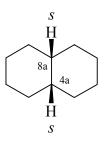


(S)-1,6-dioxaspiro[4.4]nonane

(R)-1,6-dioxaspiro[4.4]nonane >

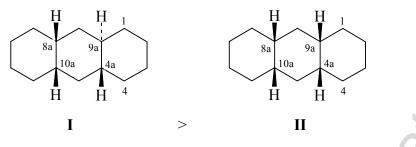


(4ar,8ar)-decahydronaphthalene



(4as,8as)-decahydronaphthalene

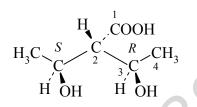
>



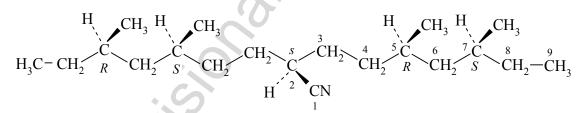
I rel-(4aR,8aR,9aR,10aS)-tetradecahydroanthracene

II rel-(4aR,8aR,9aS,10aS)-tetradecahydroanthracene

 (in the order 4a,8a,9,a,10a the stereodescriptors are 'R,R,R,S' for compound I and 'R,R,S,S' for compound II; the pairs '4a,8a' are 'R,R' (*like*) for both compounds; the pairs '4a,9a' are 'R,R' ('l') and 'R,S' (unlike), respectively; as *like* precedes unlike, compound I is senior to compound II).



(2*s*,3*R*)-3-hydroxy-2-[(*S*)-1-hydroxyethyl]butanoic acid (for the symbol '*s*' at position 2, see P-92.3.5)



(2s,5R,7S)-5,7-dimethyl-2-[(3S,5R)-3,5-dimethylheptyl]nonanenitrile (both pairs of stereodescriptors are *unlike* in sequence rule 4; as '*R*' precedes 'S' in sequence rule 5, the principal chain is chosen that has the '*R*' configuration for the chirality center encountered first along the chain)

P-45 The principal chain in substituent groups

P-45.0 Introduction

Compound acyclic substituents, i.e., substituted acyclic substituents, consist of a principal chain and one or more acyclic substituents. If the substituent to the principal chain also has acyclic substituents, it itself is a compound substituent; the resulting complete substituent is called a complex acyclic substituent. Complex substituents are named by extending the methods given below for compound substituents.

Compound substituents are named in two ways:

- (1) by using alkyl substituents (see P-29.2.1);
- (1) by using alkanyl substituents (see P-29.2.2).

Alkyl and alkanyl substituent groups have been defined in Section P-29. Simple alkyl substituent groups have their free valence(s) denoted by the suffixes 'yl', 'ylidene' or 'ylidyne' only at position 1. Simple alkanyl substituent groups have their free valence(s) denoted by the suffixes 'yl' or 'ylidene' which may be located at any position of the chain, except position 1. Both alkyl and alkanyl substituent groups can form compound substituent groups. In some cases, a compound substituent group resulting from substitution of the principal chain by alkyl or alkanyl substituent groups results in the same structure that corresponds to a simple alkanyl substituent group.

P-45.1 The principal chain

Selection of the principal chain is accomplished in accordance with the following criteria, applied successively in the order given until a decision is reached.

(a) the principal chain has the greater number of heteroatoms; this criterion is used only in method (b) of P-45.0.

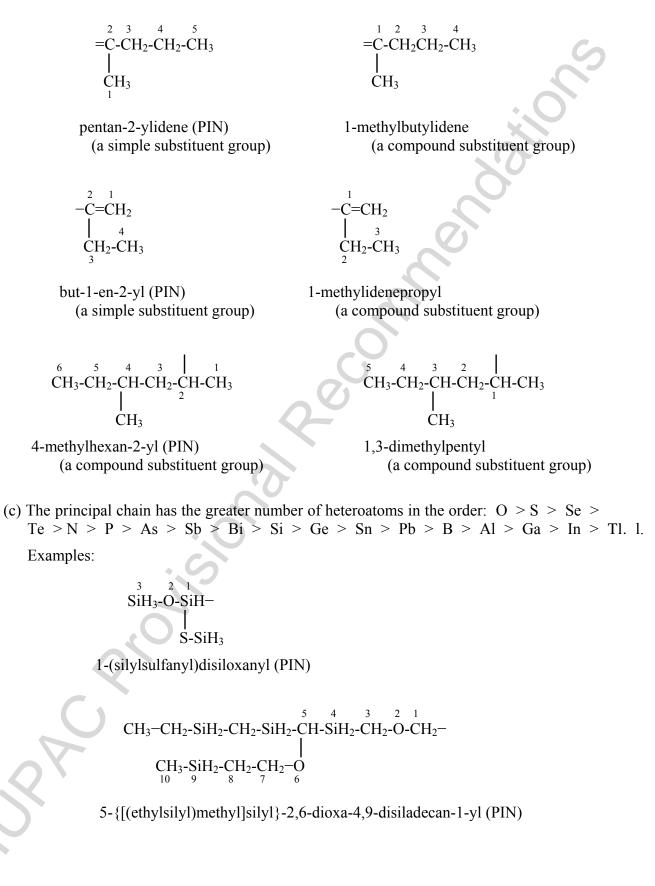
Example:

$$\begin{array}{c} 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ CH_3-SiH_2-CH-SiH_2-CH_2-SiH_2-CH_2-SiH_2-CH_2-\\ \\ \\ CH_3-CH_2-CH_2 \end{array}$$

7-propyl-2,4,6,8-tetrasilanonan-1-yl (PIN)

(b) The principal chain has the greater number of skeletal atoms, i.e., it is the longest chain; this criterion is applicable to both methods (a) and (b) of P-45.0; both methods generate simple and compound substituent groups.

Examples:



(d) The principal chain has the greater number of multiple bonds regardless of type, then the greater number of double bonds; this criterion is applicable to methods (a) and (b) in P-45.0; both generate simple and compound substituent groups.

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Examples:

hept-1-en-4-ylidene (PIN) (a simple substituent group)

$$\begin{array}{c} CH_2-CH_3\\ 1 & 2 & | & 5 & 6\\ CH_2=CH-CH-C=CH-CH_3 \end{array}$$

4-ethylhexa-1,4-dien-3-yl (PIN) (a compound substituent group)

CH₂-CH₂-CH₃

4

3 =C-CH₂-CH=CH₂

2

1-propylbut-3-en-1-ylidene (a compound substituent group)

$$CH_2-CH_3$$

$$| 3 4$$

$$CH_2=CH-CH-C=CH-CH_3$$

1-ethenyl-2-ethylbut-2-en-1-yl (a compound substituent group)

(e) The principal chain has the lowest locants for heteroatoms; this criterion is used in method (b) of P-45.0 only.

Examples:

$$\begin{array}{c} {}^{1} CH_{3} - SiH_{2} - CH_{2} - CH_{2} - SiH_{2} - CH_{2} - CH_{2} - SiH_{2} -$$

not

10 11 CH3-SiH2-CH2-CH2-SiH2-CH2-SiH2-CH2-SiH2-CH-CH2-4 5 6 7 8 2 3 CH3-CH2-SiH2-CH2-SiH2-CH2-SiH2-CH2-SiH2

10-(1,3,5,8-tetrasilanonan-10-yl)-3,5,7,9-tetrasilaundecan-11-yl (the locant set in the correct principal chain '2,5,7,9' is lower than the set '3,5,7,9')

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(f) The principal chain has the lower locant(s) for multiple bonds, regardless of type, then the lower locant(s) for double bonds; this criterion is applicable to methods (a) and (b) of P-45.0; both methods generate simple and compound substituent groups.

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Examples:

$$\begin{array}{c} 4 & 5 & 6 & 7 \\ -\text{CH-CH=CH-CH}_3 \\ 1 & 2 & 1 \\ \text{CH}_2\text{-CH=CH}_2 \end{array}$$

hepta-1,5-dien-4-yl (PIN) (a simple substituent group)

5-(prop-2-en-1-yl)octa-1,6-dien-3-yl (PIN) 1-ethenyl-3-(prop-2-en-1-yl)hex-4-en-1-yl (a compound substituent group)

(a compound substituent group)

2

CH2-CH=CH2

1-(prop-2-en-1-yl)but-2-en-1-yl

3 -CH-CH=CH-CH3

$$CH_2=CH-CH-CH_2-CH-CH=CH-CH_3$$

$$|$$

$$CH_2-CH=CH_2$$

(a compound substituent group)

(g) The principal chain has the greater number of substituents; this criterion is applicable to methods (a) and (b); both methods generate simple and compound substituent groups, respectively.

Examples:

$$\begin{array}{c} \overset{8}{\text{CH}_{3}} - \overset{7}{\text{CHCl-CHCl-CH-CH}_{2}} - \overset{6}{\text{CH}_{2}} - \overset{5}{\text{CH}_{2}} - \overset{1}{\text{CH}_{2}} - \overset{1}{\text{CH}_{3}} \\ & &$$

6,7-dichloro-5-(2-chloropropyl)octan-2-yl (PIN) (a substituted compound substituent)

$$-CH-CH_2-OH$$

$$|$$

$$CH_3$$

2-hydroxy-1-methylethyl [not 1-(hydroxymethyl)ethyl] (a substituted compound substituent group)

$$CH_{3}-CHCl-CHCl-CH-CH_{2}-CH_{2}-CH_{2}-CH_{3}-CHCl-CH_{2}-CH_{2}-CH_{2}-CH_{3}-CHCl-CH_{2}$$

5,6-dichloro-4-(2-chloropropyl-1-methylheptyl (a substituted compound substituent)

(h) The principal chain has the lowest locants for substituents; this criterion is applicable to methods (a) and (b) of P-45.0; both methods generate simple and compound substituent groups.

Examples:

$$-CH-CH(OH)-CH_{3}$$
$$| 1$$
$$CH_{2}-CH_{2}-OH$$

1,4-dihydroxypentan-3-yl (PIN) (a substituted simple substituent)

1

3 2

-CH-CH(CH₃)-CH₃ 5 CH₂-CH₂-Br

5-bromo-2-methylpentan-3-yl (PIN) (a substituted simple substituent)

CH₃-CH(OH)-CH-CH-CH₃

HO-CH₂-CH₂

pentan-2-yl (PIN)

substituent)

4-hydroxy-3-(2-hydroxyethyl)

(a substituted compound

-CH-CH(OH)-CH CH₂-CH₂-OF

2-hydroxy-1-(2-hydroxyethyl)propyl (a substituted compound substituent)

3

1 2

1-(2-bromoethyl)-2-methylpropyl (a substituted copound substituent)

$$\begin{array}{c|c} 4 & 3 & 2 \\ CH_3-CH(OH)-CH-CH-CH_3 \\ & & 1 \\ HO-CH_2-CH_2 \end{array}$$

3-hydroxy-2-(2-hydroxyethyl))-1-methylbutyl (a substituted compound substituent)

(i) The principal chain has lower locants for the substituent(s) cited earlier in alphanumerical order; this criterion is applicable to methods (a) and (b); both methods generate simple and complex substituent groups.

Examples:

$$\begin{array}{c}
3 & 2 & 1 \\
-CH-CHBr-CH_3 \\
\begin{vmatrix} & 5 \\
CHCl-CH_3 \\
4
\end{array}$$

2-bromo-4-chloropentan-3-yl (PIN) (a substituted simple substituent group) (not 4-bromo-2-chloropentan-3-yl)

2-bromo-1-(1-chloroethyl)propyl (a substituted compound substituent group) [not 1-(bromoethyl)-2-chloropropyl; 'bromo...chloro' is preferred to 'bromoethyl']

$$\begin{array}{c|c} CH_3 & CH_2-CH_3 \\ 9 & 8 & 6 & 4 & 2 & 1 \\ CH_3-CH_2-CH-CH_2-CH-CH_2-CH-CH_2-CH_3 \\ 3-ethyl-7-methylnonan-5-yl (PIN) \end{array}$$

(a compound substituent)

CH₃ CH₂-CH₃ 2 4 5 CH₃-CH₂-CH-CH₂-CH-CH₂-CH₃-CH₃-CH₃-CH₂-CH₃-CH₂-CH₃-CH₂-CH₃-CH₂-CH₃-CH₂-CH₃-CH₂-CH₃-CH₂-CH₃-CH₃-CH₂-CH₃-

3-ethyl-1-(2-methylbutyl)pentyl (a substituted compound substituent)

P-46 Substitution rules for parent structures with retained names

The following rules are used for the substitution of parent hydrides having retained names and described in P-22.1.2, P-22.1.3, Tables 2.2, 2.3, 2.7, 2.8 and Tables 3.1, 3.2 for functional parent compounds given in P-34.

Substitutability of parent structures with retained names is classified into three types:

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

- **Type 2a**. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;
- Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

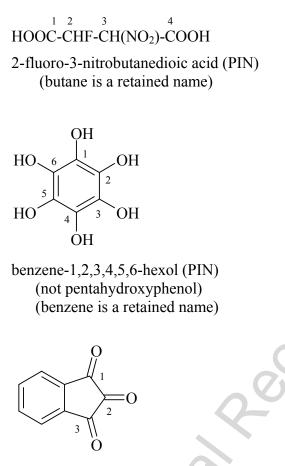
Type 2c. Substitution for parent structures not covered by Types 2a or 2b.

Type 3. Substitution of any kind not allowed

P-46.1 Type 1 substitution rules

P-46.1.1 Type 1 substitution is recommended for retained names of parent hydrides described in Chapters 2 and 3. There is no limit to the number of substituent groups cited as suffixes or prefixes, like or unlike.

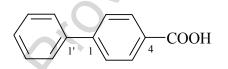
Examples:



indane-1,2,3-trione 1*H*-indene-1,2,3-trione (PIN)

P-46.1.2 Criteria to select the senior ring or ring system and the principal chain must be applied to names of all retained parent structures.

Examples:

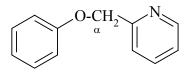


1,1'-biphenyl-4-carboxylic acid (PIN) (not 4-phenylbenzoic acid)

CH₃-CH₂-C≡CH

but-1-yne (not ethylacetylene)

butoxybenzene (PIN) (not α-propylanisole)



2-(phenoxymethyl)pyridine (PIN) [not α-(pyridin-2-yl)anisole]

P-46.2 Type 2 substitution

Substitution of parent hydrides with retained names or their derived substituent prefixes and of functional parent compounds whose names explicitly or implicitly express the presence of a characteristic group normally expressed as a suffix such as '-one', or a functional class, such as ether is limited in different ways as described in the following subsections Rules for the substitution of inorganic oxo acids used as functional parents and parent structures are described in P-67.

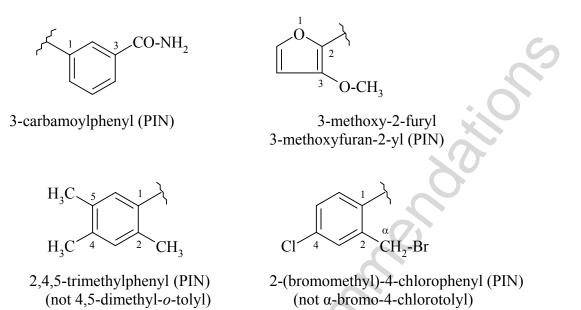
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P-46.2.1 Type 2a substitution rules

P-46.2.1.1 Type 2a includes substituent groups having free valences of any type, '-yl', 'ylidene,', 'ylidyne', 'diyl', 'ylylidene', etc. As free valences correspond to the most senior class, any substituent group is cited as a prefix.

Examples:

-CH=CH-COOH 2-carboxyvinyl 2-carboxyeth-1-en-1-yl (PIN) -CH₂-CH=CH-N(CH₃)₃ 3-(trimethylazaniumyl)allyl 3-(trimethylazaniumyl)prop-2-en-1-yl (PIN) 3-(trimethylammoniumyl)allyl



P-46.2.1.2 Type 2a includes functional parent compounds whose name expresses or implies a characteristic group normally expressed as suffix.

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P-46.2.1.2.1 Substitution by introducing substituent groups, expressed as prefixes, having lesser seniority than that denoted by the suffix is allowed.

Examples:

H₂N-CH₂-CO-CH₃

HS-CH₂-COOH

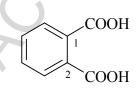
aminoacetone 1-aminopropan-2-one (PIN) 2-sulfanylacetic acid (PIN)

Furthermore, a suffix explicitly or implicitly present cannot be repeated.

Examples:

HOOC-CH₂-COOH

propanedioic acid (PIN) malonic acid (not 2-carboxyacetic acid)



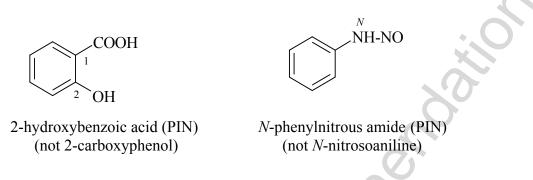
phthalic acid (PIN) (not 2-carboxybenzoic acid)

COOH HOOC COOH

benzene-1,2,4-tricarboxylic acid (PIN) (not 2,4-dicarboxybenzoic acid, nor 4-carboxyphthalic acid) P-46.2.1.2.2 The senior functional suffix or class must be expressed in the name.

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Examples:



P-46.2.2. Type 2b substitution rules

P-46.2.2.1 Type 2b includes parent compounds explicitly or implicitly devoid of suffixes. Thus, substitution of these parent compounds is possible by using compulsory prefixes only. Acetylene and allene are included in this class.

The following characteristic groups cited as compulsory prefixes can be used to substitute parent structures of Type 2b (ring and the side chain if required): halides -Br, -Cl, -F, -I, pseudohalides $-N_3$, -NCO (and chalcogen analogues), -NC, substituent groups derived from the halogen oxo acids -ClO, $-ClO_2$, $-ClO_3$ (similarly for groups in which Cl is replaced by Br or I), $-NO_2$ and -NO, $-PO_2$ and -PO, and -OR (R = alkyl groups), and chalcogen analogues. Examples:

	1 2 3
Br-C≡C-H	1 2 3 Cl-CH=C=CH-Cl
bromoacetylene (PIN)	1,3-dichloroallene (PIN)

P-46.2.3 Type 2c substitution rules apply to functional parent compounds that are not included in type 2b, for example, hydroxylamine and formic acid.

P-46.2.3.1 Substitution of hydroxylamine

Hydroxylamine can be *O*-substituted by –COOH and –SO₃OH groups, and their derived groups, that are cited as suffixes (see P-68.3.1.1.1.4).

Example:

H₂N-O-SO₃OH

 H_2N -O-CO- NH_2

hydroxylamine-O-sulfonic acid (preselected name) hydroxylamine-O-carboxamide (PIN)

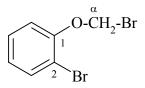
P-46.2.3.2 Substitution of anisole, toluene, benzyl, and benzylidene

The parent compound names anisole, toluene, and benzyl are retained preferred IUPAC names but cannot be substituted (see Type 3 below). However, they can be used in general

nomenclature and cannot be substituted by suffixes, only by compulsory prefixes; prefixes derived from suffix groups must lead to names expressing those prefixes as suffixes. In addition, the α -position in all of them cannot be substituted by an acyclic carbon atom which would lengthen the chain. Furthermore, anisole and toluene cannot be substituted by other methoxy or methyl groups, respectively.

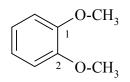
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Examples:

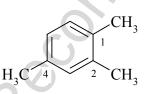


 α ,2-dibromoanisole 1-bromo-2-(bromomethoxy)benzene (PIN)

 α, α, α -trichlorotoluene (trichloromethyl)benzene (PIN)



1,2-dimethoxybenzene (PIN) (not 2-methoxyanisole)



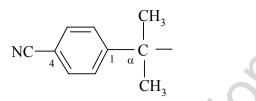
1,2,4-trimethylbenzene (PIN) (not 4-methyl-o-xylene, nor 2,4-dimethyltoluene)

O-CH₃Br O-CH₂Cl

α-bromo-2-(chloromethoxy)anisole α-phenylbenzyl [not 2-(bromomethoxy)- α -chloroanisole; bromo...chloro is alphabetically preferred unit) to bromomethoxy] 1-(bromomethoxy)-2-(chloromethoxy)benzene (PIN)

(benzyl is a larger structural diphenylmethyl (PIN)

4-methylbenzyl (not *p*-tolylmethyl; benzyl is a larger larger structural unit) (4-methylphenyl)methyl (PIN)



2-(4-cyanophenyl)propan-2-yl (PIN) 1-(4-cyanophenyl)-1-methylethyl (not 4-cyano-α,α-dimethylbenzyl)

P-46.2.3.2 Substitution rules for formic acid

The hydrogen atom attached to carbon is substitutable under specific conditions. Substitution of the hydrogen atom of formic acid by the following atoms or groups of functional replacement nomenclature, -OOH, -SH, -SeH, -TeH, -F, -Cl, -Br, -I, $-N_3$, -NC, -NCO, -NCS, -NCSe, -NCTe, $-NH_2$, leads to preferred IUPAC names derived from carbonic acid (see P-and by the $-NHNH_2$ group leads to derivatives of hydrazine (see P-). Hence, these groups cannot substitute the hydrogen atom of formic acid. However, atoms or groups not on this list may sybstitute the hydrogen atom of formic acid.

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Example:

O₂N-COOH

nitroformic acid (PIN)

P-46.3. For parent hydrides and functional parent compounds of type 3, no substitution of any kind is allowed. Functionalization of characteristic groups, such as the formation of esters, anhydrides, and salts, however, is allowed