Corrected subsections P-45.2.3 and P-45.5.1

Unfortunately the published book, the 2013 edition of *The Nomenclature of Organic Chemistry*, *IUPAC Recommendations and Preferred Names* has numerous errors, most of which are relatively minor some of which might be considered insignificant, such as a simple, obvious misspelling or an omitted closing parentheses following the descriptor PIN, as (PIN after a preferred name. However, the most serious errors occur in subsections P-45.2.3 and P-45.5.1.

Rule P-45.2.3 states "The preferred IUPAC name is based on the senior parent structure that has the lower locant or set of locants for substituents cited as prefixes to the parent structure (other than 'hydro/dehydro' prefixes) in their order of citation in the name" and

Rule P-45.5.1 states: "The preferred IUPAC name is the name that is earlier in alphanumerical order (see P-14.5). Alphabetic letters are considered first in the order that they appear in the name; all Roman letters are considered before any italic letters, unless the latter are used as locants or are a part of a compound or composite locant, for example, '*N*' and '4a'. Then, if still there is a choice, numerical locants are considered in the order of their appearance in the name."

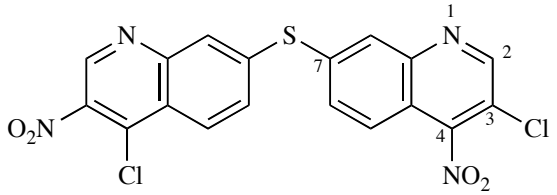
For most of the examples given in P-45.5.1 consideration was not given to the earlier hierarchical Rule P-45.2.3 where preference is given to lower locants in the order that they appear in the name.

Accordingly, Rules 45.2.3 (page 526-527) and P-45.5.1 (page 531-535) as corrected are given below.

P-45.2.3 The preferred IUPAC name is based on the senior parent structure that has the lower locant or set of locants for substituents cited as prefixes to the parent structure (other than 'hydro/dehydro' prefixes) in their order of citation in the name.

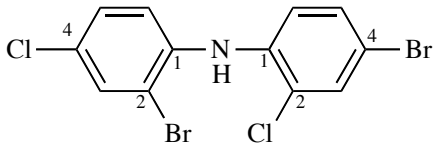
Examples:

(1)



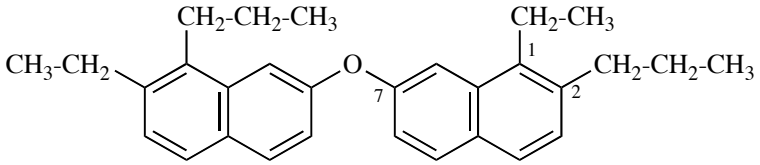
3-chloro-7-[(4-chloro-3-nitroquinolin-7-yl)sulfanyl]-4-nitroquinoline (PIN)
[not 4-chloro-7-[(3-chloro-4-nitroquinolin-7-yl)sulfanyl]-3-nitroquinoline; the locant sets are the same in both names, i.e., '3,4,7', but in their order of appearance in the name, the locant set '3,7,4' in the PIN is lower than '4,7,3']

(2)



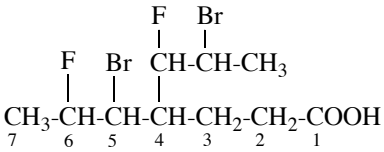
2-bromo-*N*-(4-bromo-2-chlorophenyl)-4-chloroaniline (PIN)
[not 4-bromo-*N*-(2-bromo-4-chlorophenyl)-2-chloroaniline; the locant sets are the same, i.e., '*N*,2,4' but in their order of appearance in the name the locant set '2,*N*,4' in the PIN is lower than '4,*N*,2']

(3)



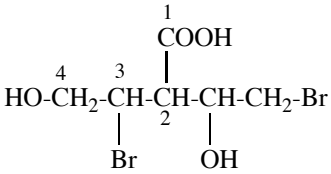
1-ethyl-7-[(7-ethyl-8-propylnaphthalen-2-yl)oxy]-2-propylnaphthalene (PIN)
[not 2-ethyl-7-[(7-ethyl-8-propylnaphthalen-2-yl)oxy]-1-propylnaphthalene; the locant sets are the same in both names, i.e., '1,2,7' but in their order of appearance in the name, the locant set '1,7, 2' in the PIN is lower than '2,7,1']

(4)



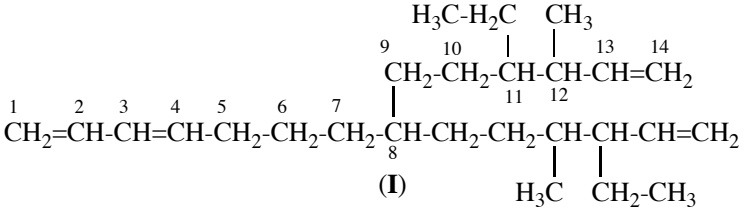
5-bromo-4-(2-bromo-1-fluoropropyl)-6-fluoroheptanoic acid (PIN)
[not 6-bromo-4-(1-bromo-2-fluoropropyl)-5-fluoroheptanoic acid; the locant sets are the same in both names, i.e., '4,5,6', but in their order of appearance in the name the locant set '5,4,6' in the PIN is lower than '6,4,5']

(5)

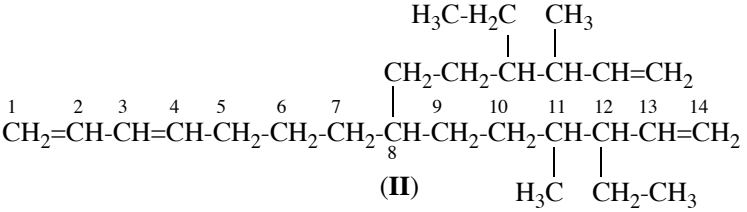


3-bromo-2-(2-bromo-1-hydroxyethyl)-4-hydroxybutanoic acid (PIN)
[not 4-bromo-2-(1-bromo-2-hydroxyethyl)-3-hydroxybutanoic acid; the locant sets are the same in both names, i.e., '2,3,4', but in their order of appearance in the name, the locant set '3,2,4' in the PIN is lower than '4,2,3']

(6)



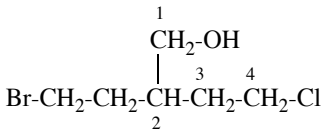
(**I**)



(**II**)

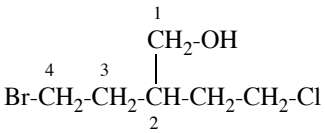
11-ethyl-8-(4-ethyl-3-methylhex-5-en-1-yl)-12-methyltetradeca-1,3,13-triene **(I)** (PIN)
[not 12-ethyl-8-(3-ethyl-4-methylhex-5-en-1-yl)-11-methyltetradeca-1,3,13-triene **(II)**; the locant sets are the same in both names, i.e., '8,11,12', but in their order of appearance in the name the locant set'11,8,12' in the PIN is lower than '12,8,11'

(7)



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

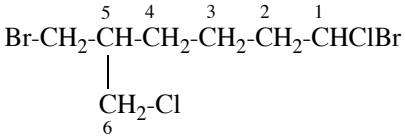
not



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

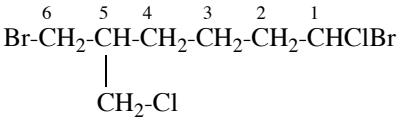
Explanation: the locant sets are the same in both names, i.e., '2,4' but in their order of appearance in the name, the locant set '2,4' in the PIN is lower than '4,2']

(8)



1-bromo-5-(bromomethyl)-1,6-dichlorohexane (PIN)

not

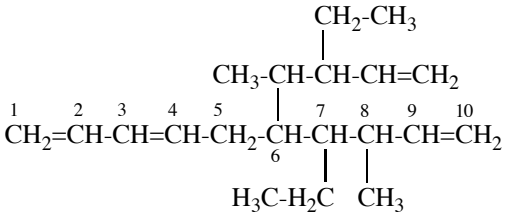


1,6-dibromo-1-chloro-5-(chloromethyl)hexane

Explanation: the locant sets are the same in both names, i.e., '1,1,5,6' but in their order of appearance in the name, the locant set '1,5,1,6' is lower than '1,6,1,5').

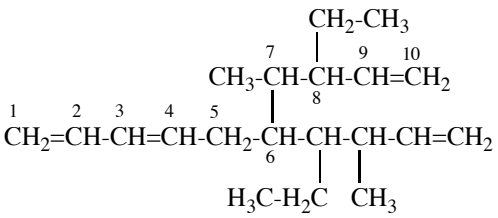
Note: Rule [C-13.11(j)] in the 1979 Recommendations (ref. 1) leads to the 'not' name)

(9)



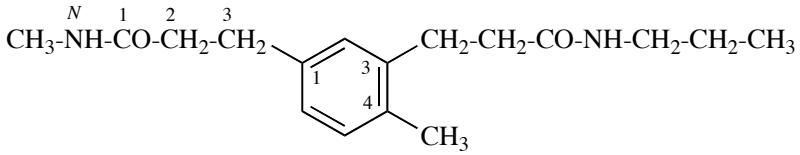
7-ethyl-6-(3-ethylpent-4-en-2-yl)-8-methyldeca-1,3,9-triene (PIN)

not

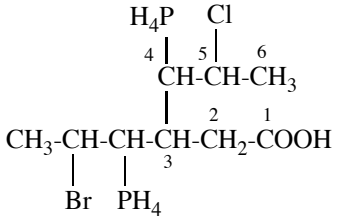


8-ethyl-7-methyl-6-(4-methylhex-5-en-3-yl)deca-1,3,9-triene

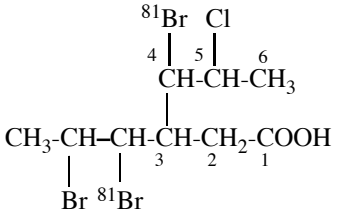
Explanation: the locant sets are the same in both names, i.e., '6,7,8' but in their order of appearance in the name, the locant set '7,6,8' is lower than '8,7,6'.

(10) 

N-methyl-3-{4-methyl-3-[3-oxo-3-(propylamino)propyl]phenyl}propanamide (PIN)
[not 3-{2-methyl-5-[3-(methylamino)-3-oxopropyl]phenyl}-*N*-propylpropanamide;
(the locant sets are the same in both names, i.e., '*N*,3' but in the order of their appearance in the PIN the locant set '*N*,3' in the PIN is lower than '3,*N*')

(11) 

3-[2-bromo-1-(λ^5-phosphanyl)propyl]-5-chloro-4-(λ^5-phosphanyl)]hexanoic acid (PIN)
[not 5-bromo-3-[2-chloro-1-(λ^5-phosphanyl)propyl]-4-(λ^5-phosphanyl)hexanoic acid;
the locant sets are the same in both names, i.e., '3,4,5' but in their order of appearance in the name, the locat set '3,5,4' in the PIN is lower than '5,3,4']

(12) 

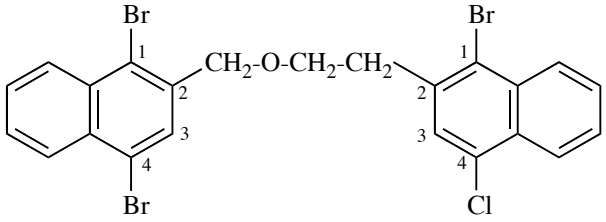
4-(^{81}Br)bromo-3-[1-(^{81}Br)bromo-2-bromopropyl]-5-chlorohexanoic acid (PIN)
[not 4-(^{81}Br)bromo-5-bromo-3-[1-(^{81}Br)bromo-2-chloropropyl]hexanoic acid; the locant sets are the same in both names, i.e., ',3,4,5' but in their order of appearance in the name, the locant set '4,3,5' in the PIN lower than '4,5,3']

P-45.5 CRITERIA RELATED TO ALPHANUMERICAL ORDER OF NAMES

P-45.5.1 The preferred IUPAC name is the name that is earlier in alphanumerical order (see P-14.5). Alphabetic letters are considered first in the order that they appear in the name; all Roman letters are considered before any italic letters, unless the latter are used as locants or are a part of a compound or composite locant, for example, '*N*' and '4a'. Then, if still there is a choice, numerical locants are considered in the order of their appearance in the name.

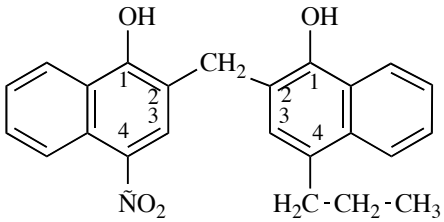
Examples:

(1)



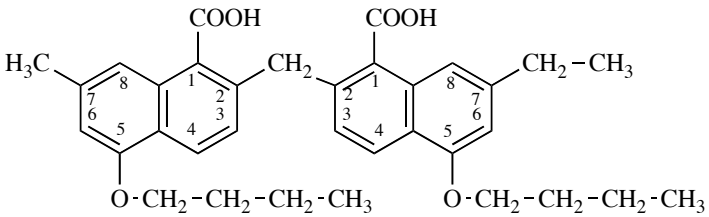
1-bromo-4-chloro-2-{2-[(1,4-dibromonaphthalen-2-yl)methoxy]ethyl}naphthalene (PIN)
[not 1,4-dibromo-2-{[2-(1-bromo-4-chloronaphthalen-2-yl)ethoxy]methyl}naphthalene;
in both names locant set is '1,2,4' and the locants appear in the name in the same order, '1,4,2', so no decision can be made by P-45.2.2 or P-45.2.3; but 'bromo' in the PIN is earlier alphabetically than 'dibromo']

(2)



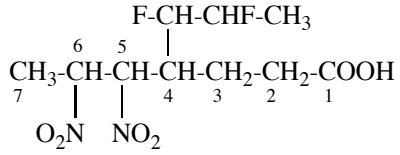
2-[(1-hydroxy-4-nitronaphthalen-2-yl)methyl]-4-propylnaphthalen-1-ol (PIN)
[not 2-[(1-hydroxy-4-propylnaphthalen-2-yl)methyl]-4-nitronaphthalen-1-ol;
in both names the lower locant set is '1,2,4' and the locants appear in the same order, '2,4,1', so no decision can be made by P-45.2.2 or P-45.2.3, but 'nitro' in the PIN is earlier alphabetically than 'propyl']

(3)



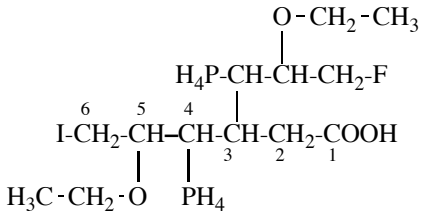
4-butoxy-2-(4-butoxy-1-carboxy-7-ethylnaphthalen-2-yl)-7-methylnaphthalene-1-carboxylic acid (PIN)
[not 4-butoxy-2-(1-carboxy-4-butoxy-7-methylnaphthalen-2-yl)-7-ethylnaphhalene-1-carboxylic acid;
in both names the lower locant set is '1,2,4,7' and the locants appear in the same order, '4,2,7,1', so no decision can be made by P-45.2.2 or P-45.2.3, but 'butoxy.....butoxy' in the PIN is earlier alphabetically than 'butoxy.....carboxy']

(4)



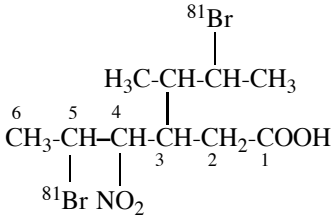
4-(1,2-difluoropropyl)-5,6-dinitroheptanoic acid (PIN)
[not 4-(1,2-dinitropropyl)-5,6-difluoroheptanoic acid;
in both names the lower locant set is '1,2,4,7' and the locants appear in the same order, '4,2,7,1', so no decision can be made by P-45.2.2 or P-45.2.3, but 'difluoropropyl' in the PIN is earlier alphabetically than 'dinitropropyl']

(5)



5-ethoxy-3-[2-ethoxy-3-fluoro-1-(λ^5-phosphanyl)propyl]-6-iodo-
4-(λ^5-phosphanyl)]hexanoic acid
{not 5-ethoxy-3-[2-ethoxy-3-iodo-1-(λ^5-phosphanyl)propyl]-6-fluoro-4-(λ^5-phosphanyl)hexanoic acid; in both names the locant set is '3,4,5,6' and the locants appear in the same order in the name, '5,3,6,4', so no decision can be made by P-45.2.2 or P-45.2.3'; but 'ethoxy...ethoxy....fluoro' in the PIN is earlier alphabetically than 'ethoxy...ethoxy....iodo'}

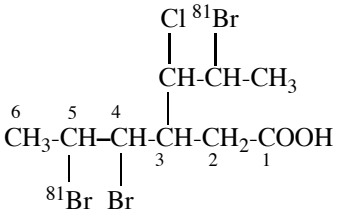
(6)



5-(^{81}Br)bromo-3-[3-(^{81}Br)bromobutan-2-yl]-4-nitrohexanoic acid (PIN)
[not 5-(^{81}Br)bromo-3-[2-(^{81}Br)bromo-1-nitropropyl]-4-methylhexanoic acid;
in both names the lower locant set is '3,4,5' and the locants appear in the same order in both names, 5,3,4', so no decision can be made by P-45.2.2 or P-45.2.3; but 'bromo...bromo...butanyl' in the PIN is lower alphabetically than 'bromo...bromo...nitro']

[**Note**: The 'B' of the element symbol 'Br' is not a factor in the alphabetization]

(7)



5-(^{81}Br)bromo-4-bromo-3-[2-(^{81}Br)bromo-1-chloropropyl]hexanoic acid (PIN)
[not 5-(^{81}Br)bromo-4-chloro-3-[2-(^{81}Br)bromo-1-bromopropyl]hexanoic acid
'bromo...bromo' is lower alphanumerically than 'bromo…chloro']

[Note: The 'B' of the element symbol 'Br is not a factor in the alphabetization]