CHAPTER 8 ISOTOPICALLY MODIFIED COMPOUNDS

P-80 Introduction

This Section describes a general system of nomenclature for organic compounds whose isotopic nuclides composition (ref. 12) deviates from that occurring in nature (for a discussion of the meaning of 'natural composition' see ref. 26). Comparative examples of the application of these rules are given in Table 8.1, page 17). This Chapter is derived from Section H of the 1979 Recommendations (ref. 1).

There is one other general system in use for describing isotopically modified compounds. It is based on an extension of the principles proposed by Boughton (see ref. 27) for designating compounds containing hydrogen isotopes and is used mainly in the Chemical Abstracts Service index nomenclature system (see ref. 28).

The system codified in these recommendations provides for recognition of various types of isotopic modifications and thus was chosen in preference to the system based on the Boughton principles.

P-81 Symbols and Definitions

P-81.1 Nuclide symbols

The symbol for denoting a nuclide in the formula and name of an isotopically modified compound consists of the atomic symbol for the element and an arabic numeral in the left superscript position indicating the mass number of the nuclide (see ref. 14).

P-81.2 Atomic symbols

The atomic symbols used in the nuclide symbol are those given in IUPAC *Nomenclature in Inorganic Chemistry* (see ref. 14). In the nuclide symbol, the atomic symbol is printed in roman type, italicized atomic symbols being reserved for letter locants, as is customary in the nomenclature of organic compounds and described in P-14.3.

For the hydrogen isotopes protium, deuterium and tritium, the nuclides symbols ^{1}H, ^{2}H, and ^{3}H, are used. The symbols D and T for ^{2}H and ^{3}H, respectively, are used, but not when other modifying nuclides are present , because this may cause difficulties in alphabetic ordering of the nuclide symbols in the isotopic descriptor. Although the symbols *d* and *t* have been used and are still used in place of ^{2}H and ^{3}H in names formed according to the Boughton system, in no other cases are lower-case letters used as atomic symbols. Therefore, the use of *d* and *t* in chemical nomenclature outside of the Boughton system is not recommended.

P-81.3 Names for hydrogen atoms and ions

The names of the hydrogen atoms and ions are as follows (see ref. 29):

		^{1}H	^{2}H	^{3}H	natural composition
atom	H	protium	deuterium	tritium	hydrogen
anion	H^-	protide	deuteride	tritide	hydride
cation	H^+	proton	deuteron	triton	hydron

P-81.4 Isotopically unmodified compounds

An isotopically unmodified compound has a macroscopic composition such that its constituent nuclides are present in the proportions occurring in nature. Its formula and name are written in the customary manner.

Examples:

CH_4	CH_3-CH_2-OH
methane (PIN)	ethanol (PIN)

P-81.5 Isotopically modified compounds

An isotopically modified compound has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that occurring in nature. Isotopically modified compounds may be classified as

(1) isotopically substituted compounds or

(2) isotopically labeled compounds

P-82 Isotopically Substituted Compounds

P-82.0 Introduction

An isotopically substituted compound has a composition such that essentially all the molecules of the compound have only the indicated nuclide at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

P-82.1 Formulas

The formula of an isotopically substituted compound is written in the usual way except that appropriate nuclides symbols are used. When different isotopes of the same element are present in the same position, common usage is to write their symbols in order of increasing mass number.

Examples:

$^{14}CH_4$ $^{12}CHCl_3$ $CH_3\text{-}CH^2H\text{-}OH$ (not $CH_3\text{-}C^2HH\text{-}OH$)

P-82.2 Names

P-82.2.1 The name of an isotopically substituted compound is formed by inserting in parentheses the nuclide symbol(s), preceded by any necessary locant(s), letters and/or numerals, before the name or preferably before the denomination of that part of the compound that is isotopically substituted. Immediately after the parentheses there is neither space nor hyphen, except that when the name, or a part of a name, includes a preceding locant, a hyphen is inserted.

When polysubstitution is possible, the number of atoms substituted is always specified as a right subscript to the atomic symbol(s), even in case of monosubstitution.

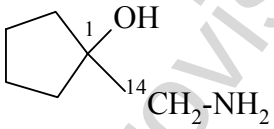
Examples:

$^{14}CH_4$
(^{14}C)methane (PIN)

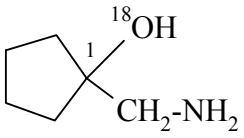
$^{12}CHCl_3$
(^{12}C)chloroform (PIN)

$CH_3{}^2H$
($^2H_1$)methane (PIN)

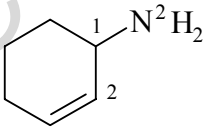
$C^2H_2Cl_2$
dichloro($^2H_2$)methane (PIN)



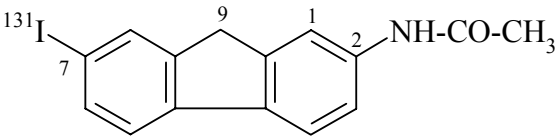
1-[amino(^{14}C)methyl]cyclopentan-1-ol (PIN)



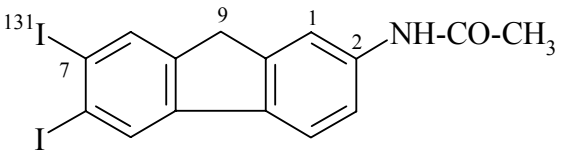
1-(aminomethyl)cyclopentan-1-(^{18}O)ol (PIN)



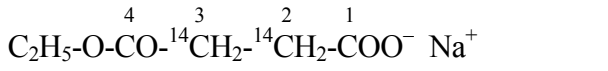
cyclohex-2-en-1-($^2H_2$)amine (PIN)



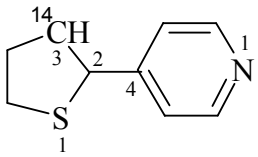
N-[7-(^{131}I)iodo-9*H*-fluoren-2-yl]acetamide (PIN)



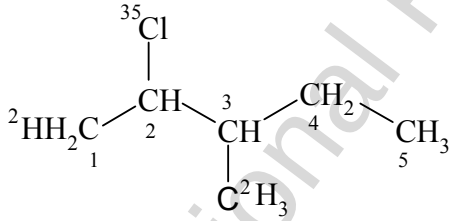
N-[6,7-(7-^{131}I)iodo-9*H*-fluoren-2-yl]acetamide (PIN)



sodium ethyl (2,3-$^{14}C_2$)butanedioate (PIN)
sodium ethyl (2,3-$^{14}C_2$)succinate



4-[(3-^{14}C)thiolan-2-yl]pyridine (PIN)
4-[tetrahydro-(3-^{14}C)-furan-2-yl]pyridine



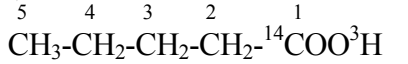
2-(^{35}Cl)chloro-3-[($^{2}H_3$)methyl](1-$^{2}H_1$)pentane (PIN)

P-82.2.2 In a name consisting of two or more words, the isotopic descriptor is placed before the appropriate word or part of the word that includes the nuclide(s), unless unambiguous locants are available or are unnecessary.

Examples:

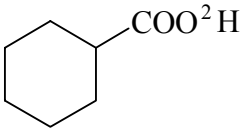
(2-$^{2}H_1$)acetic acid (PIN)

(*O*-^{2}H)acetic acid (PIN)
acetic (^{2}H)acid

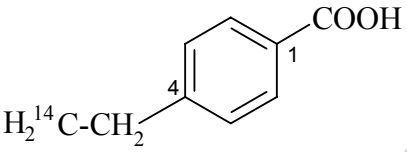


(1-^{14}C)pentan(^{3}H)oic acid (PIN)

sodium (^{14}C)formate (PIN)



cyclohexane(²H)carboxylic acid (PIN)



4-[(2-^{14}C)ethyl]benzoic acid (PIN)

CH_3-CH_2-COO-$^{14}\overset{1}{C}H_2$-$\overset{2}{C}H_3$

(1-^{14}C)ethyl propanoate (PIN)

$\overset{3}{C}H_3$-$^{14}\overset{2}{C}H_2$-$\overset{1}{C}$OO-CH_2-CH_3

ethyl (2-^{14}C)propanoate (PIN)

P-82.2.3 In a retained name or in a semisystematic name (i.e. the name of a stereoparent hydride) consisting of one word, the isotopic descriptor is placed before the name, with an appropriate locant. This method is preferred to that placing the descriptor before the implied name of the characteristic group.

Example:

$\overset{2}{C}H_3$-$\overset{1}{C}$O-$\overset{N}{N}$H²H

(*N*-²H)acetamide (PIN)
acet(²H)amide

P-82.3 Order of nuclide symbols

P-82.3.1 When isotopes of different elements are present as nuclides in a isotopically substituted, their symbols are arranged in alphabetical order if they are appear at the same place in the name.

Example:

$CH_3{}^{18}O^2H$

methan(²H,^{18}O)ol (PIN)

P-82.3.2 When several isotopes of the same element are present as nuclides, their symbols are arranged in the order of increasing mass number if they are inserted at the same place.

Example:

$\overset{2}{C}H_2$²H-$\overset{1}{C}$H³H-OH

(2-$^2H_1$,1-$^3H_1$)ethanol (PIN)

P-82.4 Stereoisomeric isotopically substituted compounds

Two types of stereoisomeric isotopically substituted compounds are possible:

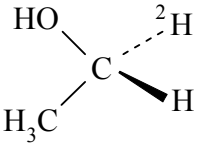
(1) those in which the stereoisomerism results from isotopic modification; and

(2) those whose analogous unmodified compounds are stereoisomers.

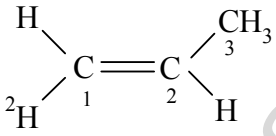
The nomenclature of stereoisomers of isotopically substituted compounds follows the general methods described in Chapter 9.

Stereochemical affixes are cited at the specified place in the name according to the stereochemical rules. When they must be inserted into the name at the same place as isotopic descriptors, the stereochemical affixes are cited first.

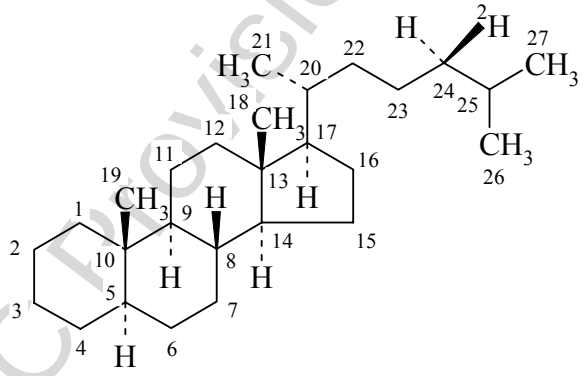
P-82.4.1 Examples in which stereoisomerism results from isotopic substitution



(R)-(1-$^{2}H_{1}$)ethanol (PIN)

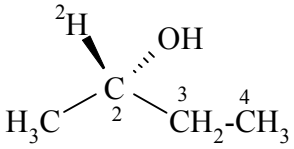


(*E*)-(1-$^{2}H_{1}$)prop-1-ene (PIN)

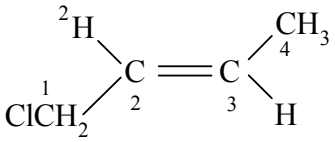


(24*R*)-5α-(24-$^{2}H_{1}$)cholestane (PIN)

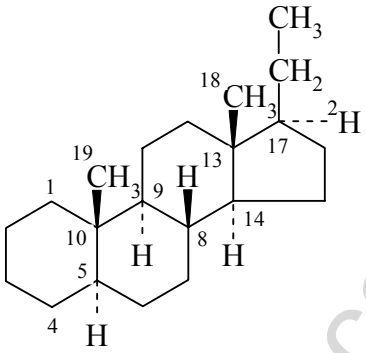
P-82.4.2 Examples of isotopically substituted stereoisomers



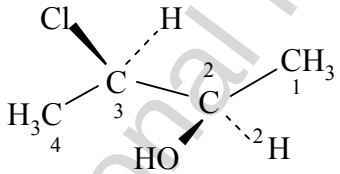
(*S*)-(2-²H)-butan-2-ol (PIN)



(*E*)-1-chloro(2-²H)but-2-ene (PIN)



5α-(17-²H)pregnane (PIN)



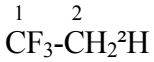
(2*R*,3*R*)-2-chloro(3-²H_1)butan-2-ol (PIN)

P-82.5 Numbering

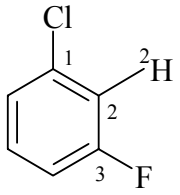
P-82.5.1 Numbering in relation to the unmodified compound

Numbering of an isotopically substituted compound is not changed from that of an isotopically unmodified compound. Among the structural features of a compound to be considered successively for numbering as given by P-14.4, the presence of nuclides is considered last with the exception of chirality arising from isotopic modification.

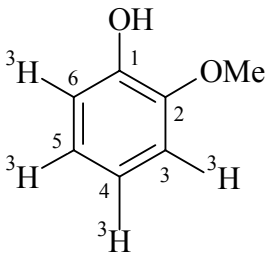
Examples:



1,1,1-trifluoro(2-²H_1)ethane (PIN)



1-chloro-3-fluoro(2-^{2}H)benzene (PIN)



2-methoxy(3,4,5,6-$^{3}H_4$)phenol (PIN)

P-82.5.2 Priority between isotopically substituted and unmodified atoms or groups

When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and the direction of numbering of the analogous isotopically substituted compound are chosen so as to give lowest locants to the modified atoms or groups considered together in one series in increasing numerical order. If a choice still remains, precedence for the lowest locants is given to the nuclide of higher atomic number. In the case of different nuclides of the same element, precedence is given to the nuclide of higher mass number.

Examples:

$^{1}CH_3$-$^{2}{}^{14}CH_2$-$^{3}CH_2$-$^{4}CH_3$

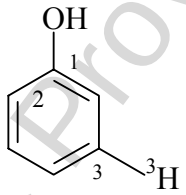
(2-^{14}C)butane (PIN)
[not (3-^{14}C)butane]

$^{1}CH_3$-$^{2}C^{2}H_2$-$^{3}{}^{14}CH_2$-$^{4}CH_3$

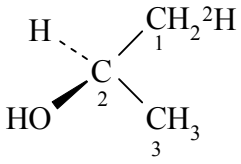
(3-^{14}C,2,2-$^{2}H_2$)butane (PIN)
[not (2-^{14}C,3,3-$^{2}H_2$)butane]

$^{1}CH_3$-$^{2}{}^{14}CH_2$-$^{3}CH^{2}H$-$^{4}CH_3$

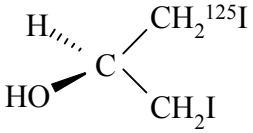
(2-^{14}C,3-$^{2}H_1$)butane (PIN)
[not (3-^{14}C,2-$^{2}H_1$)butane]



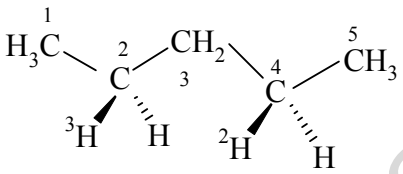
(3-^{3}H)phenol (PIN)



(*R*)-(1-$^{2}H_1$)propan-2-ol (PIN)



(*R*)-1,3-(1-^{125}I)diiodopropan-2-ol (PIN)



(2*S*,4*R*)-(4-^{2}H$_1$,2-^{3}H$_1$)pentane (PIN)

P-82.6 Locants

P-82.6.1 Omission of locants

In preferred IUPAC names, locants are omitted if no locants are necessary in unmodified names. In general nomenclature, omission may occur when no ambiguity would result.

Examples:

C^2H_3-CN

($^2H_3$)acetonitrile (PIN)
(as in trichloroacetonitrile)

CH_3-CH_2-O^{2}H

ethan(^{2}H)ol (PIN)

$CH_2{}^2H$-O-C^2H_2-S-CH_2-OOH

{[($^2H_1$)methoxy($^2H_2$)methyl]sulfanyl}methaneperoxol (PIN)

P-82.6.2 Letter and/or numeral locants

When locants are needed, all locants must be cited. Specific positions of nuclides must be indicated in the isotopic descriptor by appropriate locants, letters and/or numerals, preceding the nuclide symbol(s). In preferred names, all locants are placed before the nuclide that is multiplied accordingly.

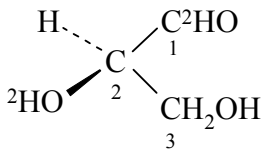
Examples:

CH_3-CH^2H-O^{2}H

(*O*,1-$^2H_2$)ethanol (PIN)
(*O*-^{2}H,1-^{2}H)ethanol

$\overset{1}{C}{}^2H_3$-$\overset{2}{C}O$-$\overset{3}{C}{}^2H_2$-$\overset{4}{C}H_2$-$\overset{5}{C}H_3$

(1,1,1,3,3-$^2H_5$)pentan-2-one (PIN)
(1-^{2}H,1-^{2}H,1-^{2}H,3-^{2}H,3-^{2}H)pentan-2-one

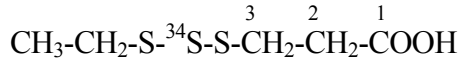


(*R*)-(2-*O*,1-²H$_2$)glyceraldehyde (PIN)
(*R*)-(2-*O*-²H,1-²H)glyceraldehyde

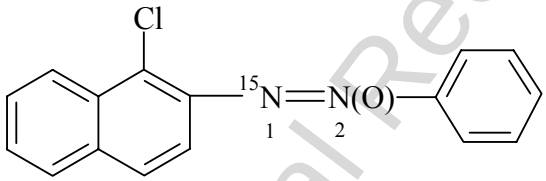
P-82.6.3 Location of nuclides on positions not normally denoted by locants

When the nuclide occupies a position that is not normally numbered, or when its position cannot be easily be defined by using the two preceding rules, the nuclide symbol may be included in the entire symbol for the group through which it is linked to the main part of the structure.

Examples:



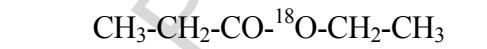
3-[ethyl(2-^{34}S)trisulfanyl]propanoic acid (PIN)



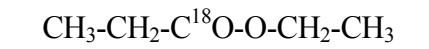
1-(1-chloro-naphthalen-2-yl)-2-phenyl(2-^{15}N)diazene 2-oxide (PIN)
2-(1-chloronaphthalen-2-yl)-1-phenyl-(2-^{15}N)-λ^5-diazen-1-one
[2-(1-chloronaphthalen-2-yl)-1-phenyl(2-^{15}N)diazen-1-ium-1-yl]oxidanide
1-chloro-2-(phenyl-*ON*^{15}*N*-azoxy)naphthalene

P-82.6.4 Italicized nuclide symbols and/or capital italic letters are used to distinguish between different nuclides of the same element.

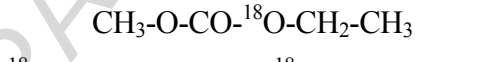
Examples:



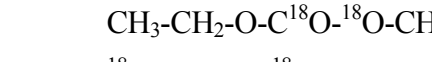
^{18}*O*-ethyl (^{18}O$_1$)propanoate (PIN)



O-ethyl (^{18}O$_1$)propanoate (PIN)



^{18}*O*-ethyl *O*-methyl (^{18}O$_1$)carbonate (PIN)



O-ethyl ^{18}*O*-methyl (^{18}O$_2$)carbonate (PIN)

P-83 Isotopically labeled compounds

An isotopically labeled compound is a mixture of isotopically unmodified compound with one or more analogous isotopically substituted compound(s).

Although an isotopically labeled compound is really a mixture as far as chemical identity is concerned (in the same way as is an unmodified compound), for nomenclature purposes, such mixtures are called 'isotopically labeled' compounds.

P-83.1 Specifically labeled compounds

An isotopically labeled compound is designated as 'specifically labeled' when a unique isotopically substituted compound is formally added to the analogous isotopically unmodified compound. In such a case, both position(s) and number of nuclides are defined.

P-83.1.1 Formulas

The structural formula of a specifically labeled compound is written in the usual way, but with the appropriate nuclide symbol(s) and multiplying subscript enclosed in square brackets, [ ]. The structural formula is written in the same way as that of an isotopically substituted compound.

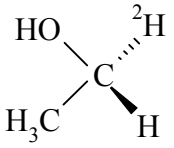
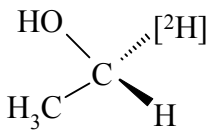
Although the formula for a specifically labeled compound does not represent the composition of the bulk material, which usually consists overwhelmingly of the isotopically unmodified compound, it does indicate the presence of the compound of chief interest, the isotopically substituted compound.

Examples:

Isotopically substituted compound	when added to	Isotopically unmodified compound	gives rise to	Specifically labeled compound
$^{13}CH_4$		CH_4		$[^{13}C]H_4$
$CH_2{}^2H_2$		CH_4		$CH_2[^2H_2]$

All structures of isotopically labeled compounds are identical to those given in Section P-8.2 for isotopically substituted compounds, but include the brackets around the nuclide.

Examples:

Formulas of isotopically substituted compounds	Formulas of specifically labeled compounds
CH_3-CO-NH^2H	CH_3-CO-NH[^{2}H]
	
C^2H_3-CO-C^2H_2-CH_2-CH_3	C[$^2H_3$]-CO-C[$^2H_2$]-CH_2-CH_3

P-83.1.1 A specifically labeled compound is

(a) singly labeled when the isotopically substituted compound has only one isotopically modified atom.

Example:

CH_3-CH[^{2}H]-OH

(b) multiply labeled when the isotopically substituted compound has more than one modified atom of the same element at the same position or at different positions.

Examples:

CH_3-C[$^3H_2$]-OH and CH_2[^{2}H]-CH[^{2}H]-OH

(c) mixed labeled when the isotopically substituted compound has more than one kind of modified atom.

Example:

CH_3-CH_2-[^{18}O][^{2}H]

P-83.1.3 Names

The name of a specifically labeled compound is formed by inserting in square brackets, [ ], the nuclide symbol(s) preceded by any necessary locants before the name or preferably before the denomination of that part of the compound that is isotopically modified. When polylabeling is possible, the number of atoms that have been labeled is always specified as a subscript to the atomic symbol(s) even in the case of monolabeling. This is necessary in order to distinguish between a specifically and a selectively or nonselectively labeled compound.

All rules given in P-10.2 to construct names of isotopically substituted compounds are applicable to construct names of specifically labeled compounds, with the exception that parentheses are used around complex prefixes when the isotopic descriptor is placed in brackets.

Examples:

$[^{13}C]H_4$

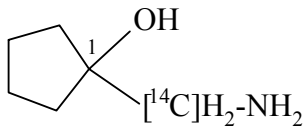
$[^{13}C]$methane (PIN)

$CH_3[^2H]$

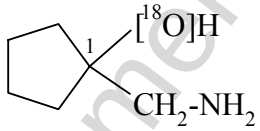
$[^2H_1]$methane (PIN)

$C[^2H_2]Cl_2$

dichloro$[^2H_2]$methane (PIN)



1-(amino$[^{14}C]$methyl)cyclopentan-1-ol (PIN)



1-(aminomethyl)cyclopentan-1-$[^{18}O]$ol (PIN)

P-83.2 Selectively labeled compounds

An isotopically labeled compound is designated as selectively labeled when a mixture of isotopically substituted compounds is formally added to the analogous isotopically unmodified compound in such a way that the position(s) but not necessarily the number of each labeling nuclide is defined. A selectively labeled compound may be considered as a mixture of specifically labeled compounds. A selectively labeled compound may be:

(a) multiply labeled when in the unmodified compound there is more than one atom of the same element at the position where the isotopic modification occurs, for example H, in CH_4; or there are several atoms of the same element at different positions where the isotopic modification occurs, for example C, in C_4H_8O;

(b) mixed labeled when there is more than one labeling nuclide in the compound, for example, C and O in CH_3-CH_2-OH.

When there is only one atom of an element that can be modified in a compound, only specific labeling can result.

P-83.2.1 Formulas

P-83.2.1.1 A selectively labeled compound cannot be described by a unique structural formula; therefore it is represented by inserting the nuclide symbol(s) preceded by any necessary locant(s) (letters and/or numbers) but without multiplying subscripts, enclosed in square brackets, [ ], directly before the usual formula or, if necessary, before parts of the formula that have an independent numbering. Identical locants are not repeated. When different nuclides are present, the nuclide symbols are written in alphabetical order according to their symbols, or when the atomic symbols are identical, in order of increasing mass number.

Examples:

Mixture of isotopically substituted compounds	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
$CH_3{}^2H$, $CH_2{}^2H_2$ CH^2H_3, C^2H_4 or any two or more of the above		CH_4		$[^2H]CH_4$
$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H^2H\text{-}\overset{1}{C}OOH$ $\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}{}^2H_2\text{-}\overset{1}{C}OOH$		$CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$		$[2\text{-}^2H]\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
$\overset{4}{C}H_3\text{-}{}^{14}\overset{3}{C}H_2\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$ $\overset{4}{C}H_3\text{-}{}^{14}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$ $\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$ or any two of the above		$CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$		$[2,3\text{-}^{14}C]\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$
$\overset{2}{C}H_3\text{-}{}^{14}\overset{1}{C}H_2\text{-}OH$ $\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}{}^{18}OH$ $\overset{2}{C}H_3\text{-}{}^{14}\overset{1}{C}H_2\text{-}{}^{18}OH$ or any two of the above		$\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$		$[1\text{-}^{14}C,{}^{18}O]\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$
$^{14}\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OO\text{-}CH_3$ $\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OO\text{-}{}^{14}CH_3$ $^{14}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OO\text{-}{}^{14}CH_3$ or any two of the above		$CH_3\text{-}CH_2\text{-}COO\text{-}CH_3$		$[3\text{-}^{14}C]\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OO\text{-}{}^{14}\overset{3}{\overset{2}{\overset{1}{C}}}]CH_3$

P-83.2.1.2 In a selectively labeled compound formally arising from mixing several known isotopically substituted compounds with the analogous isotopically unmodified compound, the number or the possible number of labeling nuclide(s) for each position may be indicated by subscripts to the atomic symbol(s).Two or more subscripts referring to the same nuclide symbol are separated by a semicolon. For a multiply labeled or mixed labeled compound, the subscripts are written successively in the same order as the various isotopically substituted compounds are considered. The subscript zero is used to indicate that one of the isotopically substituted is not modified at the indicated position.

Examples:

Mixture of isotopically substituted compounds	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
$\left.\begin{array}{l} {}^{2}CH_2{}^{2}H\text{-}{}^{1}CH_2\text{-}OH \\ {}^{2}CH^{2}H_2\text{-}{}^{1}CH_2\text{-}OH \end{array}\right]$		$CH_3\text{-}CH_2\text{-}OH$		$[2\text{-}{}^{2}H_{1;2}]{}^{2}CH_3\text{-}{}^{1}CH_2\text{-}OH$
$\left.\begin{array}{l} {}^{2}CH^{2}H_2\text{-}{}^{1}CH_2\text{-}OH \\ {}^{2}CH^{2}H_2\text{-}{}^{1}CH_2\text{-}{}^{18}OH \end{array}\right]$		$CH_3\text{-}CH_2\text{-}OH$		$[2\text{-}{}^{2}H_{2;2},{}^{18}O_{0;1}]{}^{2}CH_3\text{-}{}^{1}CH_2\text{-}OH$

P-83.2.2 Names

The name of a selectively labeled compound is formed in the same way as the name of a specifically labeled compound, except that the multiplying subscripts following the atomic symbols are generally omitted. Identical locants corresponding to the same element are not repeated. The name of a selectively labeled compound differs from the name of the corresponding isotopically substituted compound in the use of square brackets, [ ], surrounding the nuclide descriptor rather than parentheses and in the omission of repeated identical locants and multiplying subscripts.

Examples:

Mixture of isotopically substituted compounds	when added to	is named
$CH_3{}^2H$, $CH_2{}^2H_2$ CH^2H_3, C^2H_4	CH_4	[^{2}H]methane (PIN) (not [$^2H_4$]methane)
$\overset{2}{\mathbf{C}}H_3\text{-}\overset{1}{C}{}^2H_2\text{-}OH$ $\overset{2}{C}H_3\text{-}\overset{1}{C}{}^2H_2\text{-}OH$	$CH_3\text{-}CH_2\text{-}OH$	[1-^{2}H]ethanol (PIN) (not [1,1-$^2H_2$]ethanol)
$^{14}CH_3\overset{3}{\text{-}}CH_2\overset{2}{\text{-}}COO\overset{1}{\text{-}}CH_2\text{-}CH_3$ $CH_3\overset{3}{\text{-}}CH_2\overset{2}{\text{-}}COO\overset{1}{\text{-}}{}^{14}CH_2\text{-}CH_3$	$CH_3\text{-}CH_2\text{-}COO\text{-}CH_2\text{-}CH_3$	[1-^{14}C]ethyl [3-^{14}C]propanoate (PIN)
$CH_2{}^2H\overset{1}{\text{-}}CH_2\text{-}OH$ $CH^2H_2\overset{1}{\text{-}}CH_2\text{-}OH$	$CH_3\text{-}CH_2\text{-}OH$	[2-$^2H_{1;2}$]ethanol (PIN)
$CH^2H_2\overset{1}{\text{-}}CH_2\text{-}OH$ $CH^2H_2\overset{1}{\text{-}}CH_2\text{-}{}^{18}OH$	$CH_3\text{-}CH_2\text{-}OH$	[2-$^2H_{2;2}$,$^{18}O_{0;1}$]ethanol (PIN)

P-83.3 Nonselectively labeled compounds

P-83.3.1 An isotopically labeled compound is designated as nonselectively labeled when the position(s) and the number of the labeling nuclide(s) are both undefined.

When only atoms of an element to be modified are present at the same position in a compound, only specific or selective labeling can result. Nonselective labeling requires that the element to be modified be at different positions in the structure. For example, CH_4 and $CCl_3\text{-}CH_2\text{-}CCl_3$ can only be specifically or selectively labeled with a hydrogen isotope.

P-83.3.2 Formulas

Nonselective labeling is indicated in a formula by inserting the nuclide symbol, enclosed in brackets, directly before the line formula without locants or subscripts.

Example:

$[^{13}C]CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$

P-83.3.3 Names

The name of a nonselectively labeled compound is formed in the same way as the name of a selectively labeled compound but contains neither locants nor subscripts in the nuclide descriptor.

Examples:

chloro[^{3}H]benzene (PIN)

[^{13}C]glycerol (PIN)

P-83.4 Isotopically deficient compounds

P-83.4.1 An isotopically labeled compound may be designated as isotopically deficient when the isotopic content of one or more element has been depleted, i.e. when one or more nuclide(s) is(are) present in less than the natural ratio.

P-83.4.2 Formulas

Isotope deficiency is denoted in the formula by adding the italicized symbol '*def*' immediately preceding and without a hyphen, the appropriate nuclide symbol.

Example:

[*def*^{13}C]$CHCl_3$

P-83.4.3 Names

The name of an isotopically deficient compound is formed by adding the italicized symbol *def* immediately preceding and without a hyphen, the appropriate nuclide symbol, both enclosed in brackets and cited before the name or the part of the name that is isotopically modified.

Example:

trichloro[*def*^{13}C]methane (PIN)
[*def*^{13}C]chloroform

P-8.4 Comparative Examples of Formulas and Names of Isotopically Modified Compounds

Table 8.1 Comparative examples of Formulas and names of isotopically modified compounds

Types of compounds	Formula	Name
Unmodified	CH_3-CH_2-OH	Ethanol (PIN)
Isotopically substituted	C^2H_3-CH_2-O^2H	(2,2,2-$^2H_3$)ethan(^{2}H)ol (PIN) (*O*,2,2,2-$^2H_4$)ethanol (PIN)
Specifically labeled	$C[^2H_2]$-CH_2-O[^{2}H]	[2,2,2-$^2H_3$]ethan[^{2}H]ol (PIN) [*O*,2,2,2-$^2H_4$]ethanol (PIN)
Selectively labeled	[*O*,2-^{2}H]CH_3-CH_2-OH	[*O*,2-^{2}H]ethanol (PIN)
	[2-$^2H_{2;2}$,$^{18}O_{0;1}$]CH_3-CH_2-OH	[2-$^2H_{2;2}$,$^{18}O_{0;1}$]ethanol (PIN)
Nonselectively labeled	[^{2}H]CH_3-CH_2-OH	[^{2}H]ethanol (PIN)
Isotopically deficient	[*def*^{13}C]CH_3-CH_2-OH	[*def*^{13}C]ethanol (PIN)