

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

INORGANIC CHEMISTRY DIVISION

COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY*

NOMENCLATURE OF INORGANIC CHEMISTRY: II.1—ISOTOPICALLY MODIFIED COMPOUNDS

(Recommendations 1981)

Prepared for publication by

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† Deceased

NOMENCLATURE OF INORGANIC CHEMISTRY
II.1 ISOTOPICALLY MODIFIED COMPOUNDS

Approved Recommendations, 1981

PREAMBLE

These rules for the nomenclature of isotopically modified inorganic compounds (see Note b.) were developed concurrently with those for isotopically modified organic compounds[1a]. They replace Rule 1.32 of the IUPAC Inorganic Nomenclature Rules already published[2] and will be incorporated in the Third Edition of the Nomenclature of Inorganic Chemistry. The present rules presuppose naming of compounds in accordance with the provisions of the previously published rules supplementing and extending those guidelines in cases where it is desired to specify isotopic constitution.

Note a. Membership of the Commission during the preparation of these recommendations (1974-1981).

TITULAR MEMBERS: R. M. Adams (USA), 1967-1975; L. H. Bertello (Argentina), 1971-1979; D. H. Busch (USA), 1979-1983; K. Ch. Buschbeck (Federal Republic of Germany), 1971-1979; J. Chatt (UK), Chairman, 1975-1981; T. D. Coyle (USA), Secretary, 1979-1983; W. C. Fernelius (USA), 1963-1975, Chairman, 1971-1975; P. Fodor-Csányi (Hungary), 1979-1983; E. Fluck (Federal Republic of Germany), 1979-1983; Y. Jeannin (France), 1971-1981, Vice-Chairman, 1975-1981; G. J. Leigh (UK), 1973-1981; D. M. P. Mingos (UK), Secretary, 1973-1979; B. Myasoedov (USSR), 1971-1979; W. H. Powell (USA), 1975-1979; J. Reedijk (Netherlands), 1979-1983.

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†Deceased

Note b. In these rules, the term "compound" means also ions, radicals, and other species.

INTRODUCTION

These rules provide a general system of nomenclature for inorganic compounds whose isotopic nuclide[3] composition deviates from that which occurs in nature[4]. They are also suitable for designating individual isotopic molecular species. An isotopically modified organic residue occurring in an inorganic compound, such as an organic ligand in a coordination entity, is named according to the rules given in Section H of the Rules for the Nomenclature of Organic Chemistry[1a].

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 for designating compounds containing hydrogen isotopes[5], and, although mainly used in the index nomenclature of The Chemical Abstracts Service, it is found in the literature and in some chemical catalogs. This system, as it is used currently, is described elsewhere[6].

The system of nomenclature for isotopically modified inorganic compounds codified in these rules provides for recognition of various types of isotopic modification, and thus was chosen over the system based on the Boughton principles.

1.1-CLASSIFICATION AND SYMBOLISM (see Note a)

1.11-An ISOTOPICALLY UNMODIFIED COMPOUND has a macroscopic composition such that its constituent nuclides are present in the proportions occurring in nature. Its formula is written in the usual manner[2]. The name of an isotopically unmodified compound does not require alteration unless it is desired to contrast the 'natural' compound to the isotopically modified compound or to emphasize its 'natural' or 'normal' character.

Examples:

- | | |
|------------------------------|------------------------------------|
| 1. NH_3 | ammonia |
| 2. Na_2CO_3 | sodium carbonate |
| 3. HNO_3 | nitric acid |
| 4. $\text{K} [\text{AgF}_4]$ | potassium tetrafluoroargentate(1-) |
| 5. PH_3 | unmodified phosphine |
| 6. I_2O_5 | unmodified diiodine pentaoxide |

1.12-An ISOTOPICALLY MODIFIED COMPOUND has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that which occurs in nature. The formula and name of an isotopically modified compound is written according to the rules given in this chapter.

1.13-ISOTOPICALLY MODIFIED COMPOUNDS may be classified into the two broad categories: isotopically substituted compounds (see 1.2), and isotopically labeled compounds (see 1.3).

1.14-NUCLIDE SYMBOLS. The symbol for denoting a nuclide in a formula or name of an isotopically modified compound consists of the atomic symbol for the element and an Arabic number in the left superscript position which indicates the mass number of the nuclide[2a]. A metastable nuclide is indicated by adding the letter "m" to the mass number of the nuclide, e.g., $^{133\text{m}}\text{Xe}$.

1.15-ATOMIC SYMBOLS. The atomic symbols used in the nuclide symbol are those given in the IUPAC Inorganic Nomenclature Rules[2b]. In the nuclide symbol, the atomic symbol is printed in Roman type, italicized atomic symbols being reserved for letter locants, as is customary in coordination[2c] and organic[1b] chemical nomenclature.

Note a. A summary of the various types of isotopic modification is given in the Appendix.

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

1.16-ORDER OF NUCLIDE SYMBOLS. When it is necessary to cite different nuclides at the same place in the formula or name of an isotopically modified compound, the nuclide symbols are written in alphabetic order according to their atomic symbols; and when their atomic symbols are identical, in order of increasing mass number. The atomic symbols, with their locants, if any, are separated from each other by a comma.

1.2-ISOTOPICALLY SUBSTITUTED COMPOUNDS

1.21-An ISOTOPICALLY SUBSTITUTED COMPOUND has a composition such that essentially all the molecules of the compound have only the indicated nuclide(s) at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

1.22-The FORMULA OF AN ISOTOPICALLY SUBSTITUTED COMPOUND is written as usual except that appropriate nuclide symbols are used. When different nuclides of the same element are present at the same position, their symbols should be written in order of increasing mass number (see also 1.16).

1.23-The NAME OF AN ISOTOPICALLY SUBSTITUTED COMPOUND is formed by inserting in parentheses (curves) the appropriate nuclide symbol(s), preceded by any necessary locant(s) (letters and/or numerals), before the name, or preferably, before the name for 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 the name, includes a preceding locant, a hyphen is inserted.

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

When different nuclides must be cited at the same place in the name of an isotopically substituted compound, the nuclide symbols are ordered as prescribed by 1.16.

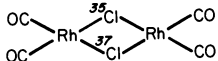
Examples:

1. H^3HO ($^3\text{H}_1$)water
2. $\text{H}_2^{15}\text{NCONH}_2$ ($^{15}\text{N}_1$)urea
3. $^{78}\text{Br}^{81}\text{Br}$ ($^{78}\text{Br}, ^{81}\text{Br}$)dibromine
4. $^2\text{H}_2^{35}\text{SO}_4$ ($^2\text{H}_2, ^{35}\text{S}$)sulfuric acid
5. Na^{36}Cl sodium (^{36}Cl)chloride
6. $^{235}\text{UF}_6$ (^{235}U)uranium hexafluoride
(^{235}U)uranium(VI) fluoride
7. $^{113\text{m}}\text{InCl}_3$ ($^{113\text{m}}\text{In}$)indium trichloride
($^{113\text{m}}\text{In}$)indium(III) chloride
($^{113\text{m}}\text{In}$)indium(3+) chloride
8. $^{15}\text{N}_2\text{O}$ di[(^{15}N)nitrogen] oxide
9. SiH_3^2H ($^2\text{H}_1$)silane
10. $^{11}\text{B}(\text{C}^2\text{H}_3)_2$ di[($^2\text{H}_3$)methoxy](^{11}B)borane
11. $\text{SiH}_2^2\text{H}-\text{SiH}^{36}\text{Cl}-\text{SiH}_3$
2-[(^{36}Cl)chloro](1- $^2\text{H}_1$)trisilane

Examples (cont.):

12. ${}^4\text{KNa}{}^{14}\text{CO}_3$ (${}^4\text{K}$)potassium sodium (${}^{14}\text{C}$)carbonate
13. $\text{Ca}_3({}^{32}\text{PO}_4)_2$ tricalcium bis[(${}^{32}\text{P}$)phosphate]
14. $\text{K}[{}^{32}\text{PF}_6]$ potassium hexafluoro(${}^{32}\text{P}$)phosphate
15. $[{}^{50}\text{Cr}({}^2\text{H}_2\text{O})_6]\text{Cl}_3$ hexa[(${}^2\text{H}_2$)aqua](${}^{50}\text{Cr}$)chromium trichloride
16. trans- $[\text{Mo}({}^{15}\text{N}_2)_2(\text{Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2)_2]$
trans-[bis[(${}^{15}\text{N}_2$)dinitrogen]bis[ethylene=
bis(diphenylphosphine)]molybdenum]

In order to retain the same name for an isotopically modified compound as for the corresponding unmodified compound as far as possible, an isotopic descriptor may be placed before a numerical prefix.

17. $\text{B}{}^{35}\text{Cl}{}^{37}\text{Cl}_2$ boron (${}^{35}\text{Cl}_1, {}^{37}\text{Cl}_2$)trichloride
(${}^{35}\text{Cl}_1, {}^{37}\text{Cl}_2$)trichloroborane
18. $\text{K}_3{}^4\text{K}[\text{Fe}(\text{CN})_6]$ (${}^4\text{K}_1$)tetrapotassium hexacyanoferrate
19.  tetracarbonyl[(${}^{35}\text{Cl}, {}^{37}\text{Cl}$)di- μ -chloro]-dirhodium

1.3 - ISOTOPICALLY LABELED COMPOUNDS

1.31-An ISOTOPICALLY LABELED COMPOUND may be considered formally as a mixture of an isotopically unmodified compound and one or more analogous isotopically substituted compounds.

NOTE: 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 a mixture is called an "isotopically labeled compound".

1.32-ISOTOPICALLY LABELED COMPOUNDS may be of various types, such as: (a) specifically labeled (see 1.33); (b) selectively labeled (see 1.34); (c) nonselectively labeled (see 1.35), and (d) isotopically deficient (see 1.36).

1.33-SPECIFICALLY LABELED COMPOUNDS

1.331-An isotopically labeled compound is called specifically labeled when a unique isotopically substituted compound is added formally to the analogous isotopically unmodified compound. In such a case, both position(s) and number of each labeling nuclide are defined.

NOTE: When free exchange among atoms of the same element in a compound occurs, e.g., H in NH_3 or in H_2NNH_2 when in contact with aqueous media, specific labeling is not possible and such isotopically labeled compounds must be considered as selectively or nonselectively labeled (see 1.34, 1.35).

1.332-The structural formula of a specifically labeled compound is written in the usual way, but with the appropriate nuclide symbol(s) and multiplying subscript, if any, enclosed in square brackets. When different nuclides of the same element are present at the same place, the nuclide symbols are ordered according to 1.16.

Examples:

<u>Isotopically substituted compound</u>	when added to:	<u>Isotopically unmodified compound</u>	results in:	<u>Specifically labeled compound</u>
H ³⁶ Cl		HCl		H[³⁶ Cl]
H ^{99m} TcO ₄		TcO ₄		H[^{99m} Tc]O ₄
³² PCl ₃		PCl ₃		[³² P]Cl ₃
Ge ² H ₂ F ₂		GeH ₂ F ₂		Ge[² H ₂]F ₂

NOTE: 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.

1.333-The name of a specifically labeled compound is formed by inserting in square brackets the nuclide symbol(s), preceded by any necessary locant(s) (letters and/or numerals), before the name or preferably before the name for that part of the compound that is isotopically modified. Immediately after the brackets there is neither space nor hyphen, except that when the name, or a part of the name, requires a preceding locant, a hyphen is inserted.

When it is possible to label more than one atom of the same element, the number of atoms that have been labeled is always specified as a right subscript to the atomic symbol(s) even when only one is labeled. This is necessary in order to distinguish between a specifically and a selectively or nonselectively labeled compound.

When different nuclides must be cited at the same place in the name of a specifically labeled compound, the nuclide symbols are ordered as given by 1.16.

The name of a specifically labeled compound differs from that of the corresponding isotopically substituted compound (see 1.23) only in the use of square brackets instead of parentheses (curves) surrounding the nuclide descriptor.

Examples:

1. H[³⁶Cl] hydrogen [³⁶Cl]chloride
2. H[^{99m}Tc]O₄ [^{99m}Tc]pertechnetate acid
hydrogen tetraoxo[^{99m}Tc]technetate(1-)
3. [³²P]Cl₃ [³²P]phosphorus trichloride
4. Ge[²H₂]F₂ difluoro[²H₂]germane
5. Na₂[³⁵S]O₃S sodium thio[³⁵S]sulfate
6. Na₂SO₃[³⁵S] sodium ([³⁵S]thio)sulfate
7. [¹⁵N]H₂[²H] [²H₁,¹⁵N]ammonia

1.334-A specifically labeled compound is (a) singly labeled when the isotopically substituted compound has only one isotopically modified atom;

Examples:

1. HO[¹⁸O]H hydrogen [¹⁸O₁]peroxide
2. H₂[¹⁵N]NH₂ [¹⁵N₁]hydrazine
3. [[⁵⁵Cr](NH₃)₆]Cl₃ hexaammine[⁵⁵Cr]chromium trichloride

(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:

1. $\text{SiH}[\text{}^2\text{H}_2]\text{-SiH}_3$ [1,1- $^2\text{H}_2$]disilane
2. $\text{Al}([\text{}^{13}\text{C}]\text{H}_3\text{-CO-}[\text{}^{13}\text{C}]\text{H-CO-}[\text{}^{13}\text{C}]\text{H}_3)_3$
tris([1,3,5- $^{13}\text{C}_3$]-2,4-pentanedionato)=
aluminum
3. $\text{Fe}(\text{CO})_2([\text{}^{13}\text{C}]\text{O})_2\text{Br}_2$ dibromo([$^{13}\text{C}_2$]tetracarbonyl)iron

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

Examples:

1. $[\text{}^{13}\text{C}]\text{O}[\text{}^{17}\text{O}]$ [^{13}C]carbon [$^{17}\text{O}_1$]dioxide
2. $[\text{}^{28}\text{Si}]\text{F}_3\text{-}[\text{}^{11}\text{B}]\text{F}_2$ difluoro(trifluoro[^{28}Si]silyl)[^{11}B]=
borane
3. $[\text{}^{32}\text{P}]\text{O}[\text{}^{18}\text{F}_3]$ [^{32}P]phosphoryl [$^{18}\text{F}_3$]fluoride
4. $\text{SiH}[\text{}^2\text{H}](\text{}^{18}\text{O})\text{CH}_3\text{-SiH}_3$ 1-([^{18}O]methoxy)[1- $^2\text{H}_1$]disilane
5. $\text{H}_2[\text{}^{10}\text{B}][\text{}^2\text{H}_2][\text{}^{10}\text{B}]\text{H}_2$ [$^{10}\text{B}_2, \mu, \mu\text{-}^2\text{H}_2$]diborane(6) (see Note a)

1.34-SELECTIVELY LABELED COMPOUNDS.

1.341-An isotopically labeled compound is called 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 isotopic modification occurs at more than one atom, either in a set of equivalent atoms at one site, e.g., H in SiH_4 , or at different sites in a molecule, e.g., B in $[\text{B}_6\text{H}_6]^{2-}$; (b) mixed labeled when there is more than one labeling nuclide in the compound, e.g., B and C in $\text{B}_8\text{C}_2\text{H}_{10}$.

NOTE: When there is only one atom of an element in a compound that can be modified, only specific labeling can result (see 1.33).

1.342-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 numerals) 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 at the same place in the formula, the nuclide symbols are ordered according to 1.16.

Note a. A more complete description would be $[\text{}^{10}\text{B}_2, (1,2-\mu), (1,2-\mu)\text{-}^2\text{H}_2]\text{diborane}(6)$ but the type of abbreviation given in this example is sufficient for simple molecules.

Examples:

<u>Mixture of isotopically substituted compounds</u>	<u>when added to:</u>	<u>Isotopically unmodified compound</u>	<u>results in:</u>	<u>Selectively labeled compound</u>
1. $\text{SOCl}^{36}\text{Cl}$ $\text{SO}^{36}\text{Cl}_2$		SOCl_2		$[\text{}^{36}\text{Cl}]\text{SOCl}_2$
2. $\text{H}_3^{32}\text{PO}_3^{18}\text{O}$ $\text{H}_3^{32}\text{PO}_4$ $\text{H}_3\text{PO}_3^{18}\text{O}$ $\text{H}_3\text{PO}_2^{318}\text{O}_2$ $\text{H}_3\text{PO}^{18}\text{O}_3$ etc.	}	H_3PO_4		$[\text{}^{18}\text{O}, \text{}^{32}\text{P}]\text{H}_3\text{PO}_4$
or any two of the above				
3. $\text{PH}_2^2\text{H}, \text{PH}^2\text{H}_2$ P^2H_3	}	PH_3		$[\text{}^2\text{H}]\text{PH}_3$
or any two of the above				
4. $\text{H}_2^{10}\text{BH}_2^{10}\text{BHCl}$ $\text{H}_2^{10}\text{BH}_2\text{BHCl}$ $\text{H}_2\text{BH}_2^{10}\text{BHCl}$	}	$\text{H}_2\text{BH}_2\text{BHCl}$		$[\text{}^{10}\text{B}]\text{B}_2\text{H}_5\text{Cl}$
or any two of the above				

NOTE: The method of writing formulas as given by the above rule may also be of use if a compound is represented by its molecular formula rather than its structural formula, e.g., $[\text{}^{1,2-2}\text{F}]\text{B}_2\text{H}_6$ rather than $[\text{}^1, \text{}^2-^2\text{H}]\text{H}_2\text{BH}_2\text{BH}_2$.

1.343-The name of a selectively labeled compound is formed in the same way as the name of a specifically labeled compound (see 1.333) except that the multiplying subscripts following the atomic symbols are generally omitted except as described in 1.344. Identical locants corresponding to the same element are not repeated.

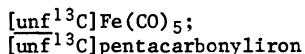
The name of a selectively labeled compound differs from the name of the corresponding isotopically substituted compound in the use of square brackets surrounding the nuclide descriptor rather than parentheses (curves) and in the omission of repeated identical locants and multiplying subscripts.

Examples:

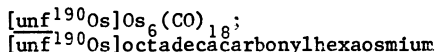
1. $[\text{}^{36}\text{Cl}]\text{SOCl}_2$	$[\text{}^{36}\text{Cl}]\text{sulfinyl chloride}$ <u>not</u> $[\text{}^{36}\text{Cl}_2]\text{sulfinyl chloride}$
2. $[\text{}^{18}\text{O}, \text{}^{32}\text{P}]\text{H}_3\text{PO}_4$	$[\text{}^{18}\text{O}, \text{}^{32}\text{P}]\text{phosphoric acid}$ <u>not</u> $[\text{}^{18}\text{O}_4, \text{}^{32}\text{P}]\text{phosphoric acid}$
3. $[\text{}^2\text{H}]\text{PH}_3$	$[\text{}^2\text{H}]\text{phosphane}$ or $[\text{}^2\text{H}]\text{phosphine}$ <u>not</u> $[\text{}^2\text{H}_3]\text{phosphane}$ or $[\text{}^2\text{H}_3]\text{phosphine}$
4. $[\text{}^{10}\text{B}]\text{H}_2\text{BH}_2\text{BHCl}$	chloro $[\text{}^{10}\text{B}]\text{diborane}(6)$ <u>not</u> chloro $[\text{}^{10}\text{B}_2]\text{diborane}(6)$
5. $[\text{}^{13}\text{C}]\text{Fe}(\text{CO})_5$	$[\text{}^{13}\text{C}]\text{pentacarbonyliron}$ <u>not</u> $[\text{}^{13}\text{C}_5]\text{pentacarbonyliron}$

Examples:

1. $[^{13}\text{C}]\text{Fe}(\text{CO})_5$ where the ^{13}C is equally distributed in each carbonyl ligand may be designated as:

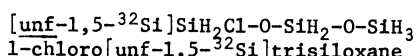


2. $[^{190}\text{Os}]\text{Os}_6(\text{CO})_{18}$ where the ^{190}Os is equally distributed among the six osmium atoms may be designated as:



The italicized descriptor unf may be followed by appropriate locants to indicate uniform labeling at specified positions.

3. $[^{32}\text{Si}]\text{SiH}_2\text{Cl-O-SiH}_2\text{-O-SiH}_3$ where the ^{32}Si is equally distributed between only the terminal silicon atoms may be designated as:



1.35-NONSELECTIVELY LABELED COMPOUNDS.

1.351-An isotopically labeled compound is called nonselectively labeled when both the position(s) and the number of labeling nuclide(s) are undefined. Nonselective labeling is indicated in the formula and name by inserting the nuclide symbol, enclosed in square brackets, directly before the usual formula or name. No preceding locants or subscripts are used.

Examples:

- | | |
|---|---|
| 1. $[^{15}\text{N}]\text{HN}_3$ | $[^{15}\text{N}]$ hydrogen azide |
| 2. $[^{32}\text{P}](\text{HO})_2\text{P}(\text{O})\text{OP}(\text{O})(\text{OH})\text{OP}(\text{O})(\text{OH})_2$ | $[^{32}\text{P}]$ triphosphoric acid |
| 3. $[^{18}\text{O}]\text{K}_4\text{H}_4\text{Si}_4\text{O}_{12}$ | tetrapotassium tetrahydrogen
$[^{18}\text{O}]$ <u>cyclo</u> -tetrasilicate |
| 4. $[^{30}\text{Si}]\text{SiH}_3\text{-SiH}_2\text{-SiH}_3$ | $[^{30}\text{Si}]$ trisilane |

1.352-Isotopically labeled nonmolecular materials, such as ionic solids and polymeric substances, where labeling nuclides may be dispersed throughout a crystal lattice or polymer network, are considered nonselectively labeled, which is designated in the formula and name according to 1.351.

Examples:

- | | |
|-----------------------------------|------------------------------------|
| 1. $[^{35}\text{Cl}]\text{NaCl}$ | $[^{35}\text{Cl}]$ sodium chloride |
| 2. $[^{235}\text{U}]\text{UO}_2$ | $[^{235}\text{U}]$ uranium dioxide |
| 3. $[^{29}\text{Si}]\text{SiO}_2$ | $[^{29}\text{Si}]$ silicon dioxide |

1.36-ISOTOPICALLY DEFICIENT COMPOUNDS. An isotopically labeled compound is called isotopically deficient when the isotopic content of one or more elements has been depleted, i.e., a nuclide is present in less than the natural ratio. An isotopically deficient compound is designated in the name and formula by adding the italicized syllable def immediately preceding, without a hyphen, to the appropriate nuclide symbol.

Examples: (see also Rule H-3.21 in Ref. [1a]).

- | | |
|---|--|
| 1. $\begin{array}{c} \text{SiHF}_2 \\ \\ \text{SiF}_3-\text{SiH}-\text{Si}[\text{}^2\text{H}]\text{F}_2 \\ \underline{1} \quad \underline{2} \quad \underline{3} \end{array}$ | 2-(difluorosilyl)-1,1,1,3,3-pentafluoro[3- $^2\text{H}_1$]trisilane
not
1-(difluoro[$^2\text{H}_1$]silyl)-1,1,1,3,3-pentafluorotrisilane |
| 2. $\begin{array}{c} \text{O}-\text{SiH}_2[\text{}^2\text{H}_1] \\ \\ \text{SiH}_2\text{Cl}-[\text{}^{18}\text{O}]-\text{SiH}-[\text{}^{18}\text{O}]-\text{SiH}_3 \\ \underline{1} \quad \underline{2} \quad \underline{3} \quad \underline{4} \quad \underline{5} \end{array}$ | 1-chloro-3-([$^2\text{H}_1$]siloxy)[2,4- $^{18}\text{O}_2$]=trisiloxane
not
1-chloro-3-([^{18}O]siloxy)[5- $^2\text{H}_1$,2- ^{18}O]=trisiloxane |
| 3. $\begin{array}{c} [\text{}^{29}\text{Si}]\text{H}_3 \\ \\ [\text{}^2\text{H}_3]\text{Si}-\text{N}-[\text{}^{30}\text{Si}]\text{H}_3 \\ \underline{1} \quad \underline{2} \quad \underline{3} \end{array}$ | 2-([^{29}Si]silyl)[1,1,1- $^2\text{H}_3$,3- ^{30}Si]=disilazane
not
2-([^{30}Si]silyl)[1,1,1- $^2\text{H}_3$,3- ^{29}Si]=disilazane |

1.43-When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and direction of numbering for the analogous isotopically modified compound are chosen so as to give the lowest locants to the modified atoms or groups considered together as one series in ascending numerical order [1d] without regard to type of nuclide or mass number. If a choice still remains, preference for lowest locants is given first to a nuclide of higher atomic number, and then to a nuclide of higher mass number.

Examples:

- | | |
|--|--|
| 1. $\begin{array}{c} \text{N}[\text{}^2\text{H}_2]-[\text{}^{15}\text{N}]\text{H}_2 \\ \underline{1} \quad \underline{2} \end{array}$ | [1,1- $^2\text{H}_2$,2- ^{15}N]hydrazine
not
[2,2- $^2\text{H}_2$,1- ^{15}N]hydrazine |
| 2. $\begin{array}{c} \text{H}_3\text{Si}-[\text{}^{29}\text{Si}]\text{H}_2-\text{SiH}[\text{}^2\text{H}]-\text{SiH}_3 \\ \underline{1} \quad \underline{2} \quad \underline{3} \quad \underline{4} \end{array}$ | [3- $^2\text{H}_1$,2- ^{29}Si]tetrasilane
not
[2- $^2\text{H}_1$,3- ^{29}Si]tetrasilane |
| 3. $\begin{array}{c} \text{H}[\text{}^{10}\text{B}] \begin{array}{l} \text{O} \\ \text{O} \end{array} \text{O}[\text{}^{11}\text{B}]\text{H} \\ \text{O}-[\text{}^{11}\text{B}]\text{H} \\ \text{O} \end{array}$ | [5- ^{10}B ,3- ^{11}B]-1,2,4,3,5-trioxa=diborolane
not
[3- ^{10}B ,5- ^{11}B]-1,2,4,3,5-trioxa=diborolane |

1.44-When isotopic modification occurs in a structure at a position that is not normally assigned a locant, group symbols or italicized prefixes may be used to denote its position.

Examples:

- | | |
|--|--|
| 1. $\text{HOSO}_2[\text{}^{35}\text{S}]\text{H}$ | [^{35}SH]thiosulfuric acid
or
[<u>mercapto</u> - ^{35}S]thiosulfuric acid |
| 2. $\text{HO}_3\text{S}[\text{}^{18}\text{O}-\text{}^{18}\text{O}]\text{SO}_3\text{H}$ | [$^{18}\text{O}-\text{}^{18}\text{O}$]peroxodisulfuric acid
or
[<u>peroxo</u> - $^{18}\text{O}_2$]peroxodisulfuric acid |

1.45-Italicized nuclide symbols and/or capital italic letters may be used as locants to distinguish between different nuclides of the same element.

Examples:

1.
$$\begin{array}{c} \text{}^{\text{18}}\text{O} \\ \parallel \\ \text{CH}_3\text{-O-P-O-CH}_3 \\ | \\ \text{O-CH}_3 \end{array}$$
 O,O,O-Trimethyl (¹⁸O₁)phosphate
2. $\text{CH}_3\text{-[}^{\text{18}}\text{O]}\text{-S(O}_2\text{)-S-CH}_3$ ¹⁸O,S-Dimethyl [¹⁸O]thiosulfate
3. $[\text{Ru}(\text{NH}_3)_5(^{\text{15}}\text{N}^{\text{14}}\text{N})]^{2+}$ pentammine[(¹⁴N,¹⁵N)dinitrogen-¹⁵N]
ruthenium(2⁺)

APPENDIX

A SUMMARY OF TYPES OF ISOTOPLICALLY MODIFIED COMPOUNDS

<u>Type of Isotopic Modification</u>	<u>Example Formula and Name</u>	<u>Explanatory Remarks</u>
Substituted	$\text{SiH}_3\text{}^2\text{H}$ (² H ₁)silane	All molecules contain one, and only one, atom of ² H.
Specifically labeled	$\text{SiH}_3\text{[}^2\text{H]}$ [² H ₁]silane	Total ² H content greater than 'natural' amount; excess H is in singly substituted molecules.
Selectively labeled	$[\text{}^1\text{-}^2\text{H}]\text{Si}_2\text{H}_6$ [¹⁻² H]disilane	Total ² H content greater than 'natural' amount; excess ² H occurs in two or more substituted molecules and may occur in any number at the specified position in a given molecule.
	$[\text{}^2\text{H}_{1;3}]\text{SiH}_4$ [² H _{1;3}]silane	Total ² H content greater than 'natural' amount; excess ² H occurs in two substituted molecules, one with one ² H atom and one with three ² H atoms.
Nonselectively labeled	$[\text{}^2\text{H}]\text{Si}_3\text{H}_8$ [² H]trisilane	Total ² H content greater than 'natural' amount; excess ² H may occur in any number and at any position in one or more substituted molecules.
Isotopically deficient	$[\text{def}^{\text{29}}\text{Si}]\text{SiHF}_3$ [<u>def</u> ²⁹ Si]trifluoro-silane	Total ²⁹ Si content is less than the 'natural' amount.

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1. International Union of Pure and Applied Chemistry, "Nomenclature of Organic Chemistry", 1979 edition; [a] Section H. Isotopically Modified Compounds, Approved Recommendations, 1978, pp. 513-538; [b] see, for example, Rule C-814.4, p. 255; [c] Rules D-4, pp. 51-59 and D-6, pp. 87-106; [d] Rule C-15.11, p. 105.
2. IUPAC, "Nomenclature of Inorganic Chemistry (1970)", 2nd ed., Butterworths, London, 1971; [a] Rule 1.31, p. 11; [b] Rule 1.1, p. 10; [c] Rule 7.33, p. 46; [d] Rule 0.33, 0.34, pp. 8-9 (Preamble) and Rule 7.72, pp. 73-4.
3. IUPAC, "Manual of Symbols and Terminology for Physicochemical Quantities and Units", 1973 ed., Butterworths, London (1975), Rules 7.1 and 7.2, p. 24.
4. For a discussion of the meaning of 'natural composition' see IUPAC, "Atomic Weights of the Elements 1979", Pure Appl. Chem., 52, 2349-2384 (1980).
5. W. A. Boughton, "Naming Hydrogen Isotopes", Science, 79, 159-60 (1934); E. J. Crane, "Nomenclature of the Hydrogen Isotopes and Their Compounds", Science, 80, 86-9 (1934); American Chemical Society, "Report of Committee on Nomenclature, Spelling, and Pronunciation, Nomenclature of the Hydrogen Isotopes and their Compounds", Ind. Eng. Chem. (News Ed.), 13, 200-1 (1935).
6. Chemical Abstracts Service, "Selection of Index Names for Chemical Substances", American Chemical Society, #220, pp. 189I-191I, a reprint of Appendix IV to the 1977 Chemical Abstracts Index Guide.
7. IUPAC, "Nomenclature of Inorganic Boron Compounds", Pure Appl. Chem., 30(3-4), 683-710 (1972).