

PROVISIONAL

INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY

INORGANIC CHEMISTRY DIVISION

COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY

NOMENCLATURE OF INORGANIC CHEMISTRY
12. ISOTOPICALLY MODIFIED COMPOUNDS

(Provisional Recommendations, 1978)

Prepared for publication by
W. C. FERNELIUS, T. D. COYLE and W. H. POWELL

Comments on these proposals should be sent within 8 months of Publication to the Secretary of the Commission:

Dr. D. M. P. MINGOS
Inorganic Chemistry Laboratory
University of Oxford
South Parks Road
Oxford OX1 3QR
UK

Comments from the viewpoint of languages other than English are encouraged. These may have special significance regarding the eventual publication in various countries of translations of the nomenclature finally approved by IUPAC.

COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY

The membership of the Commission during the preparation of these rules (1974-78) was as follows:

Chairman: W. C. Fernelius (USA), 1971-75; J. Chatt (UK), 1975-79
Vice-chairman: Y. Jeannin (France), 1975-79
Secretary: D. M. P. Mingos (UK), 1973-81

Titular Members

R. M. Adams (USA), 1967-75
L. F. Bertello (Argentina), 1971-79
K.-Ch. Buschbeck (FRG), 1971-79
Y. Jeannin (France), 1971-75
G. J. Leigh (UK), 1973-81
B. Myasoedov (USSR), 1971-79
W. H. Powell (USA), 1975-79

National Representatives

T. D. Coyle (USA), 1974-77
E. Fluck (FRG), 1975-77
P. Fodor-Csányi (Hungary), 1977-81
J. Klikorka (Czechoslovakia), 1974-77
K. Saito (Japan), 1975-77

Associate Members

R. M. Adams (USA), 1975-79
D. H. Busch (USA), 1977-81
J. Chatt (UK), 1973-75
T. D. Coyle (USA), 1977-81
T. Erdey-Grúz (Hungary)[†], 1969-76
W. C. Fernelius (USA), 1975-79
E. Fluck (FRG), 1977-81
K. A. Jensen (Denmark), 1973-81
J. Klikorka (Czechoslovakia), 1977-81
W. H. Powell (USA), 1969-75
J. Reedijk (Netherlands), 1977-81
J. Riess (France), 1973-77
K. Saito (Japan), 1977-81
E. Samuel (France), 1977-81
C. Schäffer (Denmark), 1971-79
A. A. Vlček (Czechoslovakia), 1969-77
K. Yamasaki (Japan), 1969-77

[†]Deceased

NOMENCLATURE OF INORGANIC CHEMISTRY

12. ISOTOPICALLY MODIFIED COMPOUNDS

(Provisional Recommendations, 1978)

PREAMBLE

The rules for the nomenclature of isotopically modified inorganic compounds (see Note a) proposed herein were developed concurrently with those for isotopically modified organic compounds[1] during the last five years (1974-78). They are formulated here as a new chapter to the IUPAC Inorganic Nomenclature Rules already published[2] and replace Rule 1.32 of these rules entirely. 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.

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[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 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.

12.1-CLASSIFICATION AND SYMBOLISM (see Note b)

12.11-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 |

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

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

12.12-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.

12.13-ISOTOPICALLY MODIFIED COMPOUNDS may be classified into the two broad categories: isotopically substituted compounds (see 12.2), and isotopically labeled compounds (see 12.3).

12.14-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., $^{133\text{m}}\text{Xe}$.

12.15-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[7a] chemical nomenclature.

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 d and 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 d and t outside of the Boughton system is not recommended.

12.16-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.

12.2-ISOTOPICALLY SUBSTITUTED COMPOUNDS

12.21-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.

12.22-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 12.16).

12.23-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 12.16.

Examples:

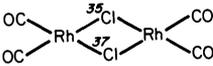
1. H^3HO ($^3\text{H}_1$)water
2. $\text{H}_2^{15}\text{NCONH}_2$ ($^{15}\text{N}_1$)urea
3. $^{78}\text{Br}^{81}\text{Br}$ ($^{78}\text{Br}, ^{81}\text{Br}$)dibromine
4. $^2\text{H}_2^{35}\text{SO}_4$ ($^2\text{H}_2, ^{35}\text{S}$)sulfuric acid

Examples (cont.):

- | | |
|--|--|
| 5. Na ³⁶ Cl | sodium (³⁶ Cl)chloride |
| 6. ²³⁵ UF ₆ | (²³⁵ U)uranium hexafluoride
(²³⁵ U)uranium(VI) fluoride |
| 7. ^{113m} InCl ₃ | (^{113m} In)indium trichloride
(^{113m} In)indium(III) chloride
(^{113m} In)indium(3+) chloride |
| 8. ¹⁵ N ₂ O | di[(¹⁵ N)nitrogen] oxide |
| 9. SiH ₃ ² H | (² H ₁)silane |
| 10. ¹¹ BH(O ² H ₃) ₂ | di[(² H ₃)methoxy](¹¹ B)borane |
| 11. SiH ₂ ² H-SiH ³⁶ Cl-SiH ₃ | 2-[(³⁶ Cl)chloro](1- ² H ₁)trisilane |
| 12. ⁴² KNa ¹⁴ CO ₃ | (⁴² K)potassium sodium (¹⁴ C)carbonate |
| 13. Ca ₃ (³² PO ₄) ₂ | tricalcium bis[(³² P)phosphate] |
| 14. K [³² PF ₆] | potassium hexafluoro(³² P)phosphate |
| 15. [⁵⁰ Cr(² H ₂ O) ₆] Cl ₃ | hexa[(² H ₂)aqua](⁵⁰ Cr)chromium trichloride |
| 16. <u>trans</u> -[Mo(¹⁵ N ₂) ₂ (Ph ₂ PCH ₂ CH ₂ PPh ₂) ₂] | <u>trans</u> -[bis[(¹⁵ 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.

Examples:

- | | |
|--|---|
| 1. B ³⁵ ClCl ³⁷ Cl | boron (³⁵ Cl ₁ , ³⁷ Cl ₁)trichloride
(³⁵ Cl ₁ , ³⁷ Cl ₁)trichloroborane |
| 2. K ₃ ⁴² K [Fe(¹⁴ CN) ₆] | (⁴² K ₁)tetrapotassium hexa[(¹⁴ C)cyano]ferrate
(⁴² K ₁)potassium hexa[(¹⁴ C)cyano]ferrate(II)
(⁴² K ₁)potassium hexa[(¹⁴ C)cyano]ferrate(4-) |
| 3.  | tetracarbonyl[(³⁵ Cl, ³⁷ Cl)di-μ-chloro]-
dirhodium |

12.3 - ISOTOPICALLY LABELED COMPOUNDS

12.31-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 mixtures are called "isotopically labeled compounds".

12.32-ISOTOPICALLY LABELED COMPOUNDS may be of various types, such as: (a) specifically labeled (see 12.33); (b) selectively labeled (see 12.34); (c) nonselectively labeled (see 12.35), and (d) isotopically deficient (see 12.36).

12.33-SPECIFICALLY LABELED COMPOUNDS

12.331-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 12.34, 12.35).

12.332-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 12.16.

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		$\text{H}[^{36}\text{Cl}]$
$\text{H}^{99\text{m}}\text{TcO}_4$		HTcO_4		$\text{H}[^{99\text{m}}\text{Tc}]_4\text{O}_4$
$^{32}\text{P}\text{Cl}_3$		PCl_3		$[^{32}\text{P}]\text{Cl}_3$
$\text{Ge}^2\text{H}_2\text{F}_2$		GeH_2F_2		$\text{Ge}[^2\text{H}_2]\text{F}_2$

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.

12.333-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 12.16.

The name of a specifically labeled compound differs from that of the corresponding isotopically substituted compound (see 12.23) only in the use of square brackets instead of parentheses (curves) surrounding the nuclide descriptor.

Examples:

- $\text{H}[^{36}\text{Cl}]$ hydrogen [^{36}Cl]chloride
- $\text{H}[^{99\text{m}}\text{Tc}]_4\text{O}_4$ [$^{99\text{m}}\text{Tc}$]pertechnetate acid
hydrogen tetraoxo [$^{99\text{m}}\text{Tc}$]technetate(1-)
- $[^{32}\text{P}]\text{Cl}_3$ [^{32}P]phosphorus trichloride
- $\text{Ge}[^2\text{H}_2]\text{F}_2$ difluoro [$^2\text{H}_2$]germane
- $\text{Na}_2 [^{35}\text{S}]\text{SO}_3$ sodium thio [^{35}S]sulfate
- $\text{Na}_2\text{S}[^{35}\text{S}]\text{O}_3$ sodium ([^{35}S]thio)sulfate
- $[^{15}\text{N}]\text{H}_2[^2\text{H}]$ [$^2\text{H}_1, ^{15}\text{N}$]ammonia

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

Examples:

1. $\text{HO}[\text{}^{18}\text{O}]\text{H}$ hydrogen $[\text{}^{18}\text{O}_1]$ peroxide
2. $\text{H}_2[\text{}^{15}\text{N}]\text{NH}_2$ $[\text{}^{15}\text{N}_1]$ hydrazine
3. $[[\text{}^{55}\text{Cr}](\text{NH}_3)_6]\text{Cl}_3$ hexaammine $[\text{}^{55}\text{Cr}]$ 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. $\text{SiH}[\text{}^2\text{H}_2]-\text{SiH}_3$ $[1,1-\text{}^2\text{H}_2]$ disilane
2. $\text{Al}([\text{}^{13}\text{C}]\text{H}_3-\text{CO}-[\text{}^{13}\text{C}]\text{H}-\text{CO}-[\text{}^{13}\text{C}]\text{H}_3)_3$
tris($[1,3,5-\text{}^{13}\text{C}_3]-2,4$ -pentanedionato)=
aluminum
3. $\text{Fe}(\text{CO})_2([\text{}^{13}\text{C}]\text{O})_2\text{Br}_2$ dibromo($[\text{}^{13}\text{C}_2]$ tetracarbonyl)iron

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

Examples:

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

12.34-SELECTIVELY LABELED COMPOUNDS.

12.341-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 12.33).

12.342-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

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

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 12.16.

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. $\text{SO}^{36}\text{ClCl}$ $\text{SO}^{36}\text{Cl}_2$		SOCl_2		$[\text{}^{36}\text{Cl}]\text{SOCl}_2$
2. $\left. \begin{array}{l} \text{H}_3^{32}\text{P}\text{O}_3^{18}\text{O} \\ \text{H}_3^{32}\text{P}\text{O}_4 \\ \text{H}_3\text{P}\text{O}_3^{18}\text{O} \end{array} \right\}$ or any two of the above		H_3PO_4		$[\text{}^{18}\text{O}, \text{}^{32}\text{P}]\text{H}_3\text{PO}_4$
3. $\left. \begin{array}{l} \text{PH}_2^2\text{H}, \text{PH}^2\text{H}_2 \\ \text{P}^2\text{H}_3 \end{array} \right\}$ or any two of the above		PH_3		$[\text{}^2\text{H}]\text{PH}_3$
4. $\left. \begin{array}{l} \text{H}_2^{10}\text{BH}_2^{10}\text{BHCl} \\ \text{H}_2^{10}\text{BH}_2\text{BHCl} \\ \text{H}_2\text{BH}_2^{10}\text{BHCl} \end{array} \right\}$ or any two of the above		$\text{H}_2\text{BH}_2\text{BHCl}$		$[\text{}^{10}\text{B}]\text{B}_2\text{H}_5\text{Cl}$

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., $[\text{}^2\text{H}]\text{B}_2\text{H}_6$ rather than $[\text{}^2\text{H}]\text{H}_2\text{BH}_2\text{BH}_2$.

12.343-The name of a selectively labeled compound is formed in the same way as the name of a specifically labeled compound (see 12.333) except that the multiplying subscripts following the atomic symbols are generally omitted except as described in 12.344. Identical locants corresponding to the same element are not repeated.

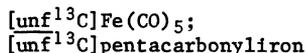
The name of a selectively labeled compound differs from the name of the corresponding isotopically substituted compound in the use of square brackets surrounding the nuclide descriptor rather than parentheses (curves) and in the omission of repeated identical locants and multiplying subscripts.

Examples:

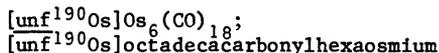
1. $[\text{}^{36}\text{Cl}]\text{SOCl}_2$	$[\text{}^{36}\text{Cl}]\text{sulfinyl chloride}$ <u>not</u> $[\text{}^{36}\text{Cl}_2]\text{sulfinyl chloride}$
2. $[\text{}^{18}\text{O}, \text{}^{32}\text{P}]\text{H}_3\text{PO}_4$	$[\text{}^{18}\text{O}, \text{}^{32}\text{P}]\text{phosphoric acid}$ <u>not</u> $[\text{}^{18}\text{O}_4, \text{}^{32}\text{P}_2]\text{phosphoric acid}$
3. $[\text{}^2\text{H}]\text{PH}_3$	$[\text{}^2\text{H}]\text{phosphine}$ or $[\text{}^2\text{H}]\text{phosphane}$ <u>not</u> $[\text{}^2\text{H}_3]\text{phosphine}$ or $[\text{}^2\text{H}_3]\text{phosphane}$

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:



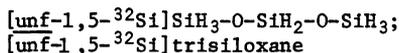
2. $[^{190}\text{Os}]_6\text{Os}_6(\text{CO})_{18}$ where the ^{190}Os is equally distributed among the six osmium atoms may be designated as:



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

Example:

1. $[^{32}\text{Si}]\text{SiH}_3\text{-O-SiH}_2\text{-O-SiH}_3$ where the ^{32}Si is equally distributed between only the terminal silicon atoms may be designated as:



12.35-NONSELECTIVELY LABELED COMPOUNDS.

12.351-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. $[^{15}\text{N}]\text{HN}_3$ | $[^{15}\text{N}]\text{hydrogen azide}$ |
| 2. $[^{32}\text{P}](\text{HO})_2\text{P}(\text{O})\text{OP}(\text{O})(\text{OH})\text{OP}(\text{O})(\text{OH})_2$ | $[^{32}\text{P}]\text{triphosphoric acid}$ |
| 3. $[^{18}\text{O}]\text{K}_4\text{H}_4\text{Si}_4\text{O}_{12}$ | tetrapotassium tetrahydrogen
$[^{18}\text{O}]\underline{\text{cyclo-tetrasilicate}}$ |
| 4. $[^{30}\text{Si}]\text{SiH}_3\text{-SiH}_2\text{-SiH}_3$ | $[^{30}\text{Si}]\text{trisilane}$ |

12.352-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 12.351.

Examples:

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

12.36-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:

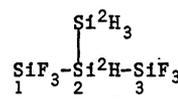
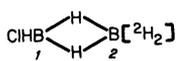
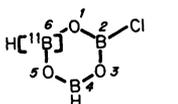
1. $[\text{def}^{10}\text{B}]\text{H}_3\text{BO}_3$ $[\text{def}^{10}\text{B}]\text{boric acid}$
 2. $[\text{def}^{235}\text{U}]\text{UF}_6$ $[\text{def}^{235}\text{U}]\text{uranium hexafluoride}$

NOTE: Commercial products are available in which one or more isotopes of an element, particularly the elements lithium, boron, uranium, and the noble gases, have been depleted. These materials do not contain the 'natural ratio' of isotopic composition and, therefore, if used for scientific research, should be so noted. In addition, certain other 'naturally occurring' materials, such as meteorites, contain elements deficient in certain nuclides, when compared to what is usually considered to be the 'natural' isotopic ratio.

12.4-LOCANTS AND NUMBERING OF ISOTOPICALLY MODIFIED COMPOUNDS

12.41-Positions of isotopic modifications in an isotopically modified compound are indicated, as far as possible, by the locants normally used for numbering of chains, rings or clusters of atoms in the corresponding unmodified compound[2d,8,9]. The assignment of locants in an isotopically modified compound should not be changed from that of the corresponding isotopically unmodified compound.

Examples:

1.  1,1,1,3,3,3-hexafluoro-2-[(²H₃)silyl]=
(2-²H₁)trisilane
3,3,3-Trifluoro-2-^{not}
(1,1,1,2-²H₄)trisilane
2.  1-chloro [2,2-²H₂]diborane(6)
2-chloro [1,1-²H₂]diborane(6)
^{not}
3.  2-chloro [6-¹¹B₁]boroxin
^{not}
6-chloro [2-¹¹B₁]boroxin

NOTE: One should be aware that when isotopically modified compounds are named by the system based on extension of the Boughton principles (see Introduction), lowest locants are assigned to isotopic positions in a 'parent' structure including unsaturation and principal groups, if any, before any other considerations. This procedure sometimes results in the assignment of higher locants to substituents expressed by prefixes, giving a numbering that differs from the one assigned by 12.41, above.

Example:



NOTE: In this example, the presence of deuterium (d) causes the silicon atom to which it is attached to be assigned the locant 1. For details and other examples, see reference[6].

12.42-When there is a choice between longest chains or a choice between equivalent rings in an isotopically unmodified compound, the preferred chain or ring of the corresponding isotopically modified compound is chosen so that the maximum number of modified atoms or groups are included. If a choice still remains, precedence is given to the chain or ring that contains first, a nuclide of higher atomic number, and then a nuclide of higher mass number.

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

- | | | |
|----|---|--|
| 1. | $\begin{array}{c} \text{SiHF}_2 \\ \\ \text{SiF}_3-\text{SiH}-\text{Si}[\text{H}^2]\text{F}_2 \\ \text{1} \quad \text{2} \quad \text{3} \end{array}$ | 2-(difluorosilyl)-1,1,1,3,3-pentafluoro[3- ² H ₁]trisilane

1-(difluoro ^{not} [² H]silyl)-1,1,1,3,3-pentafluorotrisilane |
| 2. | $\begin{array}{c} \text{O-SiH}_2[\text{H}_1] \\ \\ \text{SiH}_2\text{Cl}-[\text{O}^{18}]-\text{SiH}-[\text{O}^{18}]-\text{SiH}_3 \\ \text{1} \quad \text{2} \quad \text{3} \quad \text{4} \quad \text{5} \end{array}$ | 1-chloro-3-([² H ₁]siloxy)[2,4- ¹⁸ O ₁]=trisiloxane

1-chloro-3-([¹⁸ O]siloxy)[5- ² H ₁ ,2- ¹⁸ O ₂]=trisiloxane |
| 3. | $\begin{array}{c} [\text{Si}^{29}]\text{H}_3 \\ \\ [\text{Si}^2\text{H}_3]-\text{N}-[\text{Si}^{30}]\text{H}_3 \\ \text{1} \quad \text{2} \quad \text{3} \end{array}$ | 2-([²⁹ Si]silyl)[1,1,1- ² H ₃ ,3- ³⁰ Si ₁]=disilazane

2-([³⁰ Si]silyl)[1,1,1- ² H ₃ ,3- ²⁹ Si ₁]=disilazane |

12.43-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 [7b] 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. | $\text{N}[\text{H}_2^2]-[\text{H}_2^{15}\text{N}]_2$ | [1,1- ² H ₂ ,2- ¹⁵ N]hydrazine

^{not}
[2,2- ² H ₂ ,1- ¹⁵ N]hydrazine |
| 2. | $\text{H}_3\text{Si}_1-[\text{Si}^{29}]\text{H}_2-\text{SiH}_3[\text{H}^2]-\text{SiH}_3$ | [3- ² H ₁ ,2- ²⁹ Si]tetrasilane

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

^{not}
[3- ¹⁰ B ₁ ,5- ¹¹ B ₁]-1,2,4,3,5-trioxa=diborolane |

12.44-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. | $\text{HOSO}_2[\text{S}^{35}]\text{H}$ | [³⁵ SH]thiosulfuric acid

or
[thio- ³⁵ S]thiosulfuric acid |
| 2. | $\text{NO}_2[\text{N}^{15}]\text{H}_2$ | [¹⁵ NH ₂]nitramide

or
[amido- ¹⁵ N]nitramide |
| 3. | $[\text{N}^{15}]\text{O}_2\text{NH}_2$ | [¹⁵ NO ₂]nitramide

or
[nitro- ¹⁵ N]nitramide |
| 4. | $\text{HO}_3\text{S}[\text{O}^{180-180}]\text{SO}_3\text{H}$ | [¹⁸⁰⁻¹⁸⁰]peroxodisulfuric acid

or
[peroxo- ¹⁸⁰ O ₂]peroxodisulfuric acid |

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

Examples:

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

REFERENCES

1. IUPAC, "Nomenclature of Organic Chemistry, Section H: Isotopically Modified Compounds, Recommendations 1977", IUPAC Information Bulletin Appendices on Provisional Nomenclature, Symbols, Terminology and Conventions, No. 62, July, 1977.
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 1973", Pure Appl. Chem., 37(4), 591-603 (1974).
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 Organic Chemistry (1969)", Sections A and B, 3rd ed. (combined with Section C, 2nd ed.), Butterworths, London, 1971; [a] see, for example, Rule C-814.4; [b] Rule C-15.11, p. 105.
8. IUPAC, "Nomenclature of Organic Chemistry, Section D (Tentative)", IUPAC Information Bulletin Appendices on Tentative Nomenclature, Symbols, Units, and Standards, No. 31, August, 1973, Rule D-4, pp. 51-59; Rule D-6, pp. 87-106.
9. IUPAC, "Nomenclature of Inorganic Boron Compounds", Pure Appl. Chem., 30(3-4), 683-710 (1972).

APPENDIX

A SUMMARY OF TYPES OF ISOTOPICALLY MODIFIED COMPOUNDS

<u>Type of Isotopic Modification</u>	<u>Example Formula and Name</u>	<u>Explanatory Remarks</u>
Substituted	SiH_3^2H ($^2\text{H}_1$)silane	All molecules contain one, and only one, atom of ^2H .
Specifically labeled	$\text{SiH}_3[^2\text{H}]$ [$^2\text{H}_1$]silane	Total ^2H content greater than 'natural' amount; excess H is in single substituted molecules.
Selectively labeled	$[\text{1-}^2\text{H}]\text{Si}_2\text{H}_6$ [$1\text{-}^2\text{H}$]disilane	Total ^2H content greater than 'natural' amount; excess ^2H occurs in two or more substituted molecules and may occur in any number at the specified position in a given molecule.
	$[\text{2H}_1;_3]\text{SiH}_4$ [$^2\text{H}_1;_3$]silane	Total ^2H content greater than 'natural' amount; excess ^2H occurs in two substituted molecules, one with one ^2H atom and one with three ^2H atoms.
Nonselectively labeled	$[\text{2H}]\text{Si}_3\text{H}_8$ [^2H]trisilane	Total ^2H content greater than 'natural' amount; excess ^2H may occur in any number and at any position in one or more substituted molecules.
Isotopically deficient	$[\text{def}^{29}\text{Si}]\text{SiHF}_3$ [def^{29}Si]trifluoro-silane	Total ^{29}Si content is less than the 'natural' amount.