The Designation of Special Isotopes in the Names and Formulas of Inorganic Compounds

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RAPID EXPANSION OF THE SCIENTIFIC LITERATURE relating to work involving special isotopes of the chemical elements provides ample evidence for the need for standardization of isotope designation as an integral feature of systematic nomenclature. That the extent of use of special isotopes—both stable and radioactive—has far exceeded the expectations of some is reflected by the prophetic inaccuracy of the following statement by Otvos and Wagner which appeared only a little more than a year ago: "It is unlikely that isotopes other than deuterium will soon be available in high purity" (*Science,* October 31, 1947, p. 409).

Although some attention has been given to these matters—for example, by Otvos and Wagner (*loc. cit.*), Crane (*Science,* July 27, 1934, pp. 86–89), Dauben (private communication to Crane, January 6, 1947), and Silverman (*Chem. Eng. News,* 1947, **25**, 806)—it is only within the past year that comprehensive studies have been made in relation to the specific problem of *inorganic* substances.

Listed below are a number of recommendations and, where necessary, an indication of their limitations, some of the reasons for their adoption, etc. It should be understood at the outset that these proposals assume that the species separately designated are present in the compound in substantially isotopically pure form. For example, we are concerned primarily with the case in which $BaC^{14}O_3$ contains C^{14} almost exclusively rather than ordinary $BaCO_3$ partially enriched with respect to $BaC^{14}O_3$ or merely "spiked" with C^{14} "tracer." This does not, however, preclude the possibility of applying the rules to the latter cases provided the accompanying text makes it clear, for example, that a tracer technique is involved.

Rule 1. *In both the formulas and names of inorganic compounds, special isotopes are designated by mass numbers supplemented where necessary by the appropriate symbols.*

Implicit in this rule is the conclusion that elemental constituents not specifically designated by mass number are present in the isotopic composition of natural occurrence.

It is not considered necessary to show in either the name or the formula whether the isotope in question is stable or radioactive. Although there is much to be said in favor of relieving the reader of the need to know which isotopes are active and which are stable, both formulas and names become unduly cumbersome when an attempt is made to incorporate this and other items of information that might otherwise seem desirable.

For those cases in which isotopic mixtures other than those of natural occurrence are present, all of the appropriate mass numbers are included.

Rule 2. *In all symbols and formulas, the mass number is written as a right superscript.*

This practice represents a deviation from the recommendation included in the 1940 report of the International Union of Chemistry (Jorissen, *et al. Ber.,* 1940, **73A**, 53; *Helv. chim. Acta,* 1940, **23**, 997, 1012; *J. Amer. chem. Soc.,* 1941, **63**, 889) and emphasizes the divergence in American and European practice. The latter almost uniformly corresponds to the International Union's recommendation that mass numbers be written as left superscripts (e.g. ^{144}Pr) and that the right superscript position be reserved for its traditional indication of ionic charge or oxidation state. American practice, on the other hand, is equally uniform among both chemists and physicists, but the mass numbers are written as right superscripts (e.g. Pr^{144}).

Silverman has suggested that the mass numbers be written directly above the appropriate symbols and that the redundant nuclear charge be written below. In view of its obvious disadvantages, it seems unlikely that this suggestion will receive serious consideration.

Rule 3. *In the names of inorganic compounds, a special isotope is designated by insertion of the mass number immediately following the appropriate part of the systematic name. The mass number is set apart by a hyphen or hyphens and preceded by the corresponding symbol whenever the compound involves two constituents having overlapping ranges of mass numbers.*

In effect, it is proposed that the systematics of special isotope designation should be as nearly as possible compatible with the nomenclature practices sponsored by the International Union. The broad applicability of this general rule has been examined in relation to a large number of inorganic compounds, both simple and complex. Application of Rule 3 to a considerable number of typical cases is illustrated by the following examples:

$Fe_2{}^{59}O_3$ Iron-59(III) oxide

Where both mass number and designation of oxidation state are included, the mass number stands first.

$N_2O_4{}^{18}$ Dinitrogen tetroxide-18

Even if there were a nitrogen isotope of mass 18, the position of the mass number in the preceding name is such that it applies only to oxygen.

$Na_4{}^{24}Pb_9$	Tetrasodium-24 eannaplumbide
$Co_2{}^{58}(CO)_8$	Dicobalt-58 octacarbonyl
$Co_2(C^{14}O)_8$	Dicobalt octacarbonyl-C14
$Co_2(CO^{18})_8$	Dicobalt octacarbonyl-18

Unlike the case of dinitrogen tetroxide-18, in which the mass number is appended to that portion of the name which relates to only one component of the molecule, the last two of the preceding examples involve the name of a group consisting of two elements having contiguous ranges of mass numbers. Thus, although there is no known oxygen isotope of mass 14, the possibility of misunderstanding is decreased if the symbol for carbon is included. A still better example is provided by the cyanide group, for in this case the appended mass numbers 13 or 14 might apply to either carbon or nitrogen. Consequently, the inclusion of the symbols would be entirely necessary for clarity. While some may feel that the symbol should always accompany the mass number, maximum simplification requires that the symbol be dispensed with wherever this may be done without loss of clarity. In any borderline situations, inclusion of the symbol, even though not entirely necessary, is considered within the intent of the rule.

$Na_2V_4{}^{48}O_{11}$ Sodium tetravanadate-48

Should one choose to employ a systematic name based upon the resolved formula, one would write sodium (1:2) vanadate-48. There are undoubtedly a few instances in which the inclusion of arabic numbers for purposes other than special isotope designation might lead to difficulties, but these should be rare.

$(N^{15}H_4)_2SO_4$	Ammonium-15 sulfate
$(NH_4)_2S^{35}O_4$	Ammonium sulfate-35

Certainly neither of these two cases should cause any uncertainty with reference to the proper application of the mass numbers specified.

$Na_2SS^{35}O_3$	Sodium thio-35-sulfate
$Na_2S^{35}SO_3$	Sodium thiosulfate-35
$Na_2S_2{}^{35}O_3$	Sodium thio-35-sulfate-35

These three examples represent a case in which exchange experiments have demonstrated structurally discernible differences between like atoms (Voge and Libby. *J. Amer. chem. Soc.*, 1937, **59**, 2474; cf. Voge. *Ibid.*, 1939, **61**, 1032). Specification of the position of the special isotope requires repetition of the symbol for sulfur in the formula, while repetition of the mass number (in the name) appears desirable when the special isotope is present in both positions. With general reference to this kind of problem, it may not be anticipated that all other cases may be handled thus simply.

$K_2HP^{32}O_4$	Dipotassium hydrogen phosphate-32
$H_3PO_2S_2{}^{35}$	Dithio-35-phosphoric acid
$H_3P^{32}O_2S_2$	Dithiophosphoric-32 acid

The mass number 32 in the latter case clearly implies P^{32}, for if it were meant to apply to sulfur, the position of the mass number would be the same as in the second of the three cases.

$CaCl_2{}^{36} \cdot 8NH_3$	Calcium chloride-36 8-ammoniate
$CaCl_2{}^{36} \cdot 8N^{13}H_3$	Calcium chloride-36 8-ammoniate-13
$CaCl_2{}^{36} \cdot 8NH_3{}^2$	Calcium chloride-36 8-ammoniate-2

In the nomenclature of solvated salts it seems unlikely that the arabic numbers which show extent of solvation could lead to confusion, in view of the fact that they invariably precede rather than follow the name which indicates the nature of the solvation (*i.e.* hydrates, peroxyhydrates, ammoniates).

It will be observed that in the last of the preceding examples, specification of H^2 omits both the symbol D and the corresponding name. It is believed that the use of separate names and symbols for specific isotopes should be discouraged in every way possible. This particular hydrogen isotope is not truly a unique case in any important respect, and it may, in fact, come to assume a relatively minor role as a result of the recently announced availability of H^3. There appears to be no particular merit in the incorporation of the Boughton system (Crane, *loc. cit.*), for the nomenclature of compounds containing H^2, within the framework of systematic inorganic nomenclature.

$(CH_3)_2Ga^{72}(BH_4)$	Dimethylgallium-72 tetrahydroborate
$(CH_3)_2Ga(B^{10}H_4)$	Dimethylgallium tetrahydroborate-10
$(C^{14}H_3)_2Ga(BH_4)$	Dimethyl-14-gallium tetrahydroborate
$(CH_3{}^2)_2Ga(BH_4{}^2)$	Dimethyl-2-gallium tetrahydroborate-2

The foregoing examples provide additional applications of the general rule and include a case in which a special isotope is present in two different positions in the same molecule.

$K[Au^{198}(OH)_4]$	Potassium tetrahydroxoaurate-198(III)
$K[Au^{198}(O^{18}H^3)_4]$	Potassium tetrahydroxo-18,3-aurate-198(III)
$Fe_4^{59}[Fe(CN)_6]_3$	Iron-59 hexacyanoferrate(II)
$Fe_4[Fe^{59}(CN)_6]_3$	Iron hexacyanoferrate-59(II)
$Fe_4[Fe(C^{14}N)_6]_3$	Iron hexacyano-C14-ferrate(II)
$Fe_4[Fe(CN^{14})_6]_3$	Iron hexacyano-N14-ferrate(II)
$Fe_4^{59}[Fe^{59}(C^{14}N^{14})_6]_3$	Iron-59 hexacyano-C14,N14-ferrate-59(II)
$[Cr_3^{52}(C_2H_3O_2)_6(OH^2)_2]Br$	Hexaacetatodihydroxo-2-trichromium-52(III) bromide
$[Cr_3^{52}(C_2H_3^2O_2)_6(OH)_2]Br$	Hexaacetato-2-dihydroxotrichromium-52(III) bromide
$[Cr_3(C_2H_3^2O_2)_6(OH^3)_2]Br$	Hexaacetato-2-dihydroxo-3-trichromium(III) bromide

These examples show applicability of the rule to somewhat more complex inorganic compounds, including some extreme cases involving a degree of substitution of special isotopes unlikely to be encountered.

Rule 4. *Partial substitution by a special isotope is indicated by application of the foregoing rules, inclusion of the appropriate symbol, and insertion of a suitable coefficient specifying the extent of substitution.*

In the case of dimethylgallium tetrahydroborate, for example, suppose that there is only a partial substitution of H^2 for ordinary hydrogen, *i.e.*

$$(CH_2H^2)_2Ga(BHH_3^2).$$

The appropriate name is: Dimethyl-1H2-gallium tetrahydroborate-3H2. Although this procedure becomes unwieldy when unduly extended, it may prove useful also as a scheme for the designation of percentage enrichment with respect to a particular isotope.

Rule 5. *Wherever it is necessary to specify both mass number and ionic charge, the symbol together with the mass number as a right superscript is enclosed in parentheses and followed by the usual charge designation.*

The necessity for this rule obviously follows from the practice implicit in Rule 2. The following cases are typical:

$(Sn^{113})^{++++}$ $(Sn^{113})^{+4}$ $(Sn^{113})^{IV}$	Tin-113(IV) ion
$(U^{235}O_2)^{++}$	Uranium-235 dioxy(II) ion
$(S^{31})^{=}$	Sulfide-31 ion
$(BiO_3^{15})^{-}$	Bismuthate-15 ion

In this connection it is worthy of note that the need for both Rule 2 and Rule 5 would be obviated if American scientists would adopt the practice of writing the mass numbers as left superscripts.

Rule 6. *Metastable nuclear species are denoted by appending the lower-case letter m to the mass number.*

This practice is merely an adaptation of that employed by Seaborg and Perlman (*Rev. mod. Phys.*, in press). In the absence of the letter m, the ground state is, of course, implied. The following are typical cases:

$HgBr_2^{80m}$	Mercury(II) bromide-80m
$In_2^{115m}(SO_4)_3$	Indium-115m(III) sulfate

It is clearly evident that there will arise numerous special cases which will require modification and/or extension of these proposals. Just as is true of systematic nomenclature uncomplicated by the problem of special isotopes, it is inevitable that situations not amenable to the application of any set of rules will be encountered. In extreme cases, recourse must be had to the abandonment of names in favor of formulas; in some instances structural formulas may be required for an unequivocal designation of the position of a particular isotope. On the other hand, undue reliance should not be placed upon either the use of elaborate formulas or the possible clarification provided by the accompanying text. Tabulations and indexes should be kept as free as possible from annoying explanatory footnotes.

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