

UNCLASSIFIED



3 4456 0360885 2

ORNL 1084  
Chemistry

*8w*

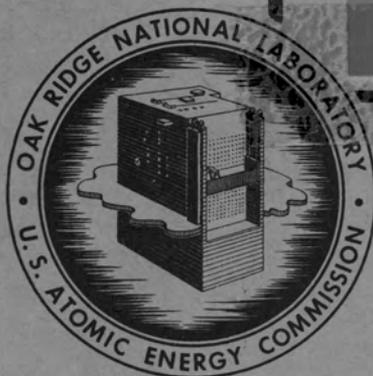
THE NOMENCLATURE OF ORGANIC  
COMPOUNDS CONTAINING ISOTOPIC CARBON

CENTRAL RESEARCH LIBRARY  
DOCUMENT COLLECTION

**LIBRARY LOAN COPY**

DO NOT TRANSFER TO ANOTHER PERSON

If you wish someone else to see this  
document, send in name with document  
and the library will arrange a loan.



OAK RIDGE NATIONAL LABORATORY  
OPERATED BY  
CARBIDE AND CARBON CHEMICALS COMPANY  
A DIVISION OF UNION CARBIDE AND CARBON CORPORATION

**UCC**

POST OFFICE BOX P  
OAK RIDGE, TENNESSEE

UNCLASSIFIED

UNCLASSIFIED

ORNL 1084  
Chemistry

This document consists of 22  
pages. No. 8 of 244 copies.  
Series A.

Contract No. W 7405 Eng 26

CHEMISTRY DIVISION

THE NOMENCLATURE OF ORGANIC COMPOUNDS  
CONTAINING ISOTOPIC CARBON

Clair J. Collins  
Charles E. Crompton  
Anthony R. Ronzio  
Bert M. Tolbert

Date Issued

---

OAK RIDGE NATIONAL LABORATORY  
operated by  
CARBIDE AND CARBON CHEMICALS COMPANY  
A Division of Union Carbide and Carbon Corporation  
Post Office Box P  
Oak Ridge, Tennessee

UNCLASSIFIED



3 4456 0360885 2

## UNCLASSIFIED

ii

ORNL 1084  
Chemistry

## INTERNAL DISTRIBUTION

- |                              |                       |                         |
|------------------------------|-----------------------|-------------------------|
| 1. G. T. Felbeck (C&CCC)     | 21. S. C. Lind        | 36. J. A. Wethington    |
| 2-3. Chemistry Library       | 22. F. C. VonderLage  | 37. C. J. Collins       |
| 4. Physics Library           | 23. R. C. Briant      | 38. A. R. Ronzio        |
| 5. Biology Library           | 24. J. A. Swartout    | 39. B. M. Tolbert       |
| 6. Health Physics Library    | 25. F. L. Steahly     | 40. M. J. Skinner       |
| 7. Metallurgy Library        | 26. A. H. Snell       | 41. E. J. Dowling       |
| 8-9. Training School Library | 27. A. Hollaender     | 42. W. J. Skraba        |
| 10-13. Central Files         | 28. M. T. Kelley      | 43. A. J. Weinberger    |
| 14. C. E. Center             | 29. K. Z. Morgan      | 44. A. R. Jones         |
| 15. C. E. Larson             | 30. J. S. Felton      | 45. D. N. Hess          |
| 16. W. B. Humes (K-25)       | 31. A. S. Householder | 46. J. G. Burr          |
| 17. W. D. Lavers (Y-12)      | 32. C. S. Harrill     | 47. G. A. Ropp          |
| 18. A. M. Weinberg           | 33. C. E. Winters     | 48. V. F. Raaen         |
| 19. E. H. Taylor             | 34. D. W. Cardwell    | 49. O. K. Neville       |
| 20. E. D. Shipley            | 35. E. M. King        | 50. <i>Central file</i> |

## EXTERNAL DISTRIBUTION

- 51-58. Argonne National Laboratory
- 59. Armed Forces Special Weapons Project
- 60-64. Atomic Energy Commission, Washington
- 65. Battelle Memorial Institute
- 66. Brush Beryllium Company
- 67-70. Brookhaven National Laboratory
- 71. Bureau of Medicine and Surgery
- 72. California Institute of Technology (R. F. Bacher)
- 73-76. Carbide and Carbon Chemicals Company (K-25 Plant)
- 77-80. Carbide and Carbon Chemicals Company (Y-12 Area)
- 81. Columbia University (G. Failla)
- 82. Dow Chemical Company
- 83-87. E. I. du Pont de Nemours and Company
- 88-93. General Electric, Richland
- 94-97. Idaho Operations Office
- 98-99. Iowa State College
- 100. Kellex Corporation
- 101-104. Knolls Atomic Power Laboratory
- 105-129. Los Alamos Scientific Laboratory
- 130. Mallinckrodt Chemical Works
- 131. Massachusetts Institute of Technology (A. Gaudin)
- 132. Massachusetts Institute of Technology (A. R. Kaufmann)
- 133-135. Mound Laboratory
- 136. National Advisory Committee for Aeronautics

UNCLASSIFIED

- 137. National Bureau of Standards (R. D. Huntoon)
- 138. Naval Medical Research Institute
- 139-140. Naval Radiological Defense Laboratory
- 141. New Brunswick Laboratory
- 142-144. New York Operations Office
- 145. North American Aviation, Inc.
- 146. Patent Branch, Washington
- 147. RAND Corporation
- 148. Sandia Corporation
- 149. Savannah River Operations Office (Wilmington)
- 150. Sylvania Electric Products, Inc.
- 151-165. Technical Information Service, Oak Ridge
- 166-167. U. S. Geological Survey (T. B. Nolan)
- 168-169. U. S. Public Health Service
- 170. U. S. Testing Company, Hoboken, New Jersey (C. E. Crompton)
- 171. University of California at Los Angeles
- 172-196. University of California Radiation Laboratory
- 197-198. University of Rochester
- 199. University of Washington
- 200. Western Reserve University
- 201-202. Westinghouse Electric Corporation
- 203-207. Atomic Energy Commission, Isotopes Division (Mr. McCormick)
- 208-211. Atomic Energy Project, Chalk River
- 212. Chief of Naval Research
- 213. H. K. Ferguson Company
- 214. Harshaw Chemical Corporation
- 215-216. Library of Congress, Acquisition Department (J. W. Corrn)
- 217. National Bureau of Standards (Library)
- 218. National Research Council, Ottawa
- 219. Naval Research Laboratory
- 220-221. Oak Ridge Institute of Nuclear Studies
- 222-231. United Kingdom Scientific Mission (M. Greenhill)
- 232. USAF, Eglin Air Force Base (Technical Library)
- 233. USAF, Wright-Patterson Air Force Base (Rodney Nudenberg)
- 234-238. USAF, Wright-Patterson Air Force Base (CADO)
- 239. U. S. Army, Army Medical Service Graduate School  
(Col. W. S. Stone)
- 240. U. S. Army, Atomic Energy Branch (Lt. Col. A. W. Betts)
- 241-243. U. S. Army, Technical Command (Col. J. H. Rothschild,  
Attention: Technical Library)
- 244. UT-AEC Agricultural Research Program (Charles S. Hobbs)

# THE NOMENCLATURE OF ORGANIC COMPOUNDS CONTAINING ISOTOPIC CARBON

By Clair J. Collins<sup>(1a)</sup>, Charles E. Crompton<sup>(1b)</sup>, Anthony R. Ronzio<sup>(1c)</sup> and  
Bert M. Tolbert<sup>(1d)</sup>

- 
- (1a) Oak Ridge National Laboratory, Chemistry Division, Oak Ridge, Tennessee.  
(1b) Formerly of the U. S. Atomic Energy Commission, Isotopes Division, Oak Ridge, Tennessee, present address, U. S. Testing Company, Hoboken, New Jersey.  
(1c) Los Alamos Scientific Laboratory, Los Alamos, New Mexico.  
(1d) Radiation Laboratory, University of California, Berkeley, California.
- 

## I. Introduction

The recent availability of the carbon isotopes with masses of 11, 13 and 14 has resulted in the synthesis of a great number of carbon-labeled<sup>(2)</sup> organic

- 
- (2) The word "labeled" is used in this paper to indicate an alteration in the isotopic composition of one or more positions in the structure of a compound so that the compound, or the positions may later be identified.
- 

compounds. The designation of these compounds by names which indicate the positions of labeling has caused much confusion. Although this problem has received some attention<sup>(3,4,5,6)</sup> in recent years, no uniform system of naming these compounds

- 
- (3) J. W. Otvós and C. D. Wagner, *Science*, 106, 409 (1947).  
(4) M. Calvin, et al. "Isotopic Carbon," Page X, John Wiley and Sons, New York, N. Y. (1949).  
(5) R. C. Anderson, Brookhaven Conference Report, Chemistry Conference #4, BNL-44 (C-10), p. 110-129, January, 1950.  
(6) C. J. Collins, *J. Am. Chem. Soc.*, 70, 2418 (1948) Footnote (3).
- 

now exists. One finds, for example, in the literature of the past two years the terms <sup>11</sup>C-formaldehyde"; "<sup>11</sup>C<sub>1</sub>-formaldehyde"; "formaldehyde-C<sub>1</sub><sup>14</sup>"; "radioformaldehyde" and

"formaldehyde-C<sup>14</sup>" all meant to designate C<sup>14</sup>H<sub>2</sub>O. As the labeled compound increases in complexity, the names given it become more numerous. Many authors have encouraged a non-systematic nomenclature by the use of such terms as "benzoic acid-carboxyl-C<sup>14</sup>," while others have described labeled compounds by the use of wordy descriptions.

The formula of an organic compound is a written symbol indicating the chemist's concept of its structure, while conveying to the observer certain of its chemical and physical properties. The expression in words of the facts represented by the formula presents many problems. A naming system by which the complete sense of every formula could be expressed would be too complicated to be of use in the coding and indexing of compounds. Possibly for this reason the naming of organic compounds has followed several trends, each of which has resulted in a unique method of notation. The criteria for naming organic compounds by each of these methods are rigorous, although the chemist may use the system of his choice, - for example (1) the Beilstein system, (2) the radical system, (3) the I. U. C. system and (4) the indexing system employed by Chemical Abstracts. The latter nomenclature is one of expedience, and the editors of Chemical Abstracts do not hesitate to borrow from other systems, to change their preferences, to establish new rules, nor to combine features of two or more systems for ease and clarity of indexing. In such a field as chemical nomenclature, in which new problems and conditions must be met continuously, the ability to cope with new requirements is essential, and a rigid and immobile system is, in fact, undesirable.

Owing to the general lack of uniformity in naming labeled compounds, the authors believe it profitable to report the result of a study they have made of the nomenclature of the compounds of isotopic carbon; this study was undertaken to achieve uniformity in their preparation of reports for the Atomic Energy Commission.

Its purpose was to examine the problems which made it difficult to name the compounds of isotopic carbon, and to point out established principles which might serve as a guide for naming these compounds in future reports. In the present study, the authors placed on themselves the following restrictions:

- (1) To suggest no new rules, symbols nor conventions.
- (2) To propose only such names as can be justified on the basis of existing precedents and good usage.
- (3) To signify no preference regarding points of controversy. The recommendations for solving such controversies are properly considered to be a function of the committee on Nomenclature of Compounds Containing Isotopic Elements, under the Chairmanship of Dr. Wallace R. Brode. This committee is advisory to the committee on Nomenclature of the Organic Division of the American Chemical Society.

Since these problems have been discussed freely with so many chemists, it is not possible to give proper credit for many of the ideas contained in the report. The advice and the many suggestions made however, by Professor Charles D. Hurd of Northwestern University, are gratefully acknowledged.

## II. Problems Involved

Most attempts to use a systematic nomenclature for purposes of naming compounds containing isotopic carbon are adaptations of the rules and precedents

established for the names of compounds containing deuterium and tritium<sup>(7,8)</sup>.

---

- (7) The proposal of W. A. Boughton reported by E. J. Crane, Ind. Eng. Chem. News Edition, 13, 200-201 (1935).
- (8) A. M. Patterson, L. T. Capell, and M. A. Magill, Chemical Abstracts, 39, 5874-5875 (1945).
- 

In names of compounds containing carbon-14, for example, the isotope symbol is usually " $C^{14}$ ", the position of the carbon-14 is usually indicated by a number or a Greek letter called a locant, and the number of positions occupied by carbon-14 atoms is shown by the use of a subscript. To illustrate, "butane-2,3- $C^{14}_2$ " signifies butane whose labeled molecules possess carbon-14 in both the 2- and 3- positions. This is a typical name for this compound, although as has been pointed out, authors are not uniform in their usage of such names.

A rigorous adaptation of the rules for deuterium and tritium nomenclature<sup>(7,8)</sup> to the naming of compounds containing isotopic carbon is difficult because of the following facts:

- (1) The letters d for deuterium and t for tritium are special symbols for the isotopes of hydrogen signifying atomic weights of two and three for this element. An extension of this system to the isotopes of all elements would obviously be undesirable.
  - (2) The numbering systems now in use for organic structures, - with the notable exception of that proposed by Dyson<sup>(9)</sup>, - refer to the substituent
- 

- (9) G. M. Dyson, "A New Notation and Enumeration System for Organic Compounds," London, New York, Longman, Green (1949).
-

at the position in a molecule rather than to the position itself. This single fact leads to at least two difficulties when these numbering systems are employed to designate the position or positions occupied by isotopic carbon:

- a. The same numbering system must be used in two different senses to indicate the positions of a substituent and isotopic carbon in the same structure. This becomes evident when one considers the meanings of the numbers in the names "2-chloroethanol-2-C<sup>14</sup>," "2-methyl-1,4-naphthoquinone-2-C<sup>14</sup>" and "2-(chloro-Cl<sup>35</sup>)-ethanol-2-C<sup>14</sup>."
- b. Many names for organic structures do not carry a complete numbering pattern. This makes it impossible to use such names when the unnumbered position or positions are the points of labeling. Consider, for example, acetic acid and its derivatives. The methyl group referred to by the name "acetic acid" has been designated the  $\alpha$ -position, but no designation either numerical or alphabetical was given for the carboxyl group. In the synonym "ethanoic acid" the carboxyl carbon is numbered as one. The American Chemical Society Committee on Nomenclature, Spelling and Pronunciation, in differentiating the two acids CH<sub>2</sub>DCOOH and CH<sub>3</sub>COOD<sup>(7)</sup> proposes the name "acetic-d acid" for the former and "acetic acid-d" for the latter. No ambiguity exists here, for when "acetic acid-d" is converted to the ethyl ester, the "OD" group is displaced. In like manner "acetic-d acid" on conversion to the ethyl ester becomes ethyl acetate-d. It is

obvious that this type of name cannot be applied to the similar cases of acetic acid labeled with isotopic carbon. In a recent ruling<sup>(10)</sup> of the I. U. C., it has been stated that the Geneva

---

(10) International Union of Pure and Applied Chemistry, September, 1949 Meeting, Amsterdam.

---

type numbering would be used with the trivial names of open chain acids, the carboxyl group being designated as the No. 1 position and the  $\alpha$ -position as the No. 2 position. This problem, therefore, may be considered as partially solved for the open-chain acids. However, the same cannot be said for many trivial names of more complex compounds. The names "desoxybenzoin" and "chalcone" for example, carry no complete numbering pattern and are inadequate for the purposes of expressing labeling with isotopic carbon in the carbonyl-groups of the structures they represent. Many such names, in fact do not lend themselves readily for designating other kinds of substitution.

- (3) The position of the locant (number or English or Greek letter) and isotope symbol in the names of compounds containing isotopic carbon has been accepted generally as a suffix by analogy to usage in deuterium and tritium names, although a few authors employ these as a prefix. Patterson<sup>(11)</sup> states "where shall position number be

---

(11) Austin M. Patterson, J. Am. Chem. Soc., 55, 3925 (1933).

---

placed, before or after the parts of the name to which they refer? Usage varies; some chemists place them before, some place them after, some use a combination. The committee  $\int$  on the Reform of Organic Nomenclature  $\int$  has left full latitude on this point." What Patterson has said indicates that the matter be left to individual preference.

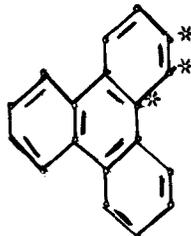
- (4) The use of carrier-free isotope as contrasted with carrier containing isotope will lead to a different species or mixture<sup>(12)</sup> of species

(12) The components of the mixture considered here are species of the same compound, differing only in their position or positions of labeling<sup>(2)</sup>.

when employed in the same synthetic series. This type of problem has been recognized<sup>(3,5)</sup> also for the compounds of deuterium and tritium. Acetylene, prepared from barium carbide which had been obtained by the action on barium of pure carbon- $C^{14}$  dioxide (containing none of the other isotopes of carbon) would contain no other species than  $C^{14}H \equiv C^{14}H$ . The use of carbon- $C^{14}$  dioxide containing both carbon- $C^{12}$  and carbon- $C^{14}$  yields mixtures of  $C^{14}H \equiv C^{14}H$ ,  $C^{14}H \equiv C^{12}H$  and  $C^{12}H \equiv C^{12}H$ . There is obviously carbon- $C^{14}$  dioxide of such a  $C^{14}/C^{12}$  ratio that the acetylene prepared from it would contain a negligible amount of the doubly-labeled species when compared to the singly-labeled acetylene. When the ratio  $C^{14}H \equiv C^{14}H / C^{14}H \equiv C^{12}H$  becomes less than the experimental error in radioactive assay employed to determine the amount

of carbon-14 in the acetylene, then that acetylene is effectively singly-labeled, even though the amount of doubly-labeled acetylene may be calculated, or even determined directly by mass-spectrographic data. The problem here is: how shall such mixtures be named?

- (5) The chemical substitution of compounds containing many identical positions, and labeled in one or more of these positions leads to complex mixtures<sup>(12)</sup> which are difficult to name without omitting some of the information that should be included in the name. Consider the hydrocarbon triphenylene containing carbon-14 in the 3-, 4- and 4a-positions. Monosubstitution of this labeled



hydrocarbon by bromine in the 2-position and all equivalent positions should yield a mixture of monobromo derivatives containing bromine at the 2-, 3-, 6-, 7-, 10- and 11-positions. The same mixture could be considered also as composed of 2-bromotriphenylenes labeled with carbon-14 in the 3-, 4-, 4a-positions, the 4b-, 5-, 6-positions, the 7-, 8-, 8a-positions, the 8b, 9-, 10-positions, the 11-, 12-, 12a-positions, and the 12a-, 1-, 2-positions. The problem is to name the bromo derivative in such a way that if the bromine were removed, one could determine from that name the positions of labeling

in the regenerated triphenylene.

III. Principles Used as a Guide for Naming Compounds  
Containing Isotopic Carbon

The following principles have been found by the present authors to provide a simple, workable nomenclature guide. Most compounds containing isotopic carbon can be named by this system. Its limitations are chiefly those of chemical nomenclature in general, since it suggests no symbols nor conventions which are not in accordance with established organic nomenclature.

- (1) Capital C rather than lowercase c is used to denote carbon isotopes. Superscripts follow, rather than precede the elemental symbol. This latter practice is apparently contrary to the convention recommended by the I. U. C. Committee on Inorganic Nomenclature<sup>(13)</sup>. In the opinion of

---

(13) Chem. and Eng. News Edition, 27, 2998 (1949).

---

the present authors however, this I. U. C. recommendation was made for the convenience of inorganic chemists in placing the charge to the upper right of the isotope symbol when writing equations for ionic reactions.

At least two cogent reasons may be advanced for non-adherence to this recommendation. First, scientists speak of, and think of "carbon-thirteen", "carbon-fourteen" and "iodine-one-thirty-one", for example, rather than "thirteen-carbon", "fourteen-carbon" and "one-thirty-one-iodine." Thus, reversal of the superscripts to "<sup>13</sup>C", "<sup>14</sup>C" and "<sup>131</sup>I"

is awkward and, for some, confusing. Second, the use of such symbols as " $C^{13}$ ", " $C^{14}$ " and " $T^{131}$ " is a convention well established by usage in the scientific literature, and has been common practice among chemists in writing symbols for the isotopes of most elements<sup>(7)</sup>.

A reversal of this usage will be difficult to effect. Since the I. U. C. recommendation has not yet been made a part of a definitive report, it is felt that non-adherence to it is entirely justified.

- (2) Consistent with deuterium and tritium nomenclature<sup>(7,8)</sup> the isotope symbol directly follows the part of the name to which it refers. The subscripts are used, as in the names of compounds which contain deuterium and tritium, to describe the number of given isotopic atoms present in a molecule or molecular moiety referred to by the isotope symbol. It should be noted however that the placing of the isotope symbol and its locant before the name or part of the name to which it refers is not incorrect<sup>(11)</sup>. There may be certain names, in fact, in which the latter practice should be preferred.
- (3) The names selected must represent correct usage within the system chosen. The formula  $(CH_3)_3COH$ , for example could be named "2-methyl-2-propanol, "t-butyl alcohol" or "trimethylcarbinol." In similar fashion, "desoxybenzoin," "phenyl benzyl ketone" or " $\alpha$ -phenylacetophenone" may be used for  $C_6H_5CH_2COC_6H_5$ . To represent isotopic substitution it is obvious that the system chosen must be capable of designating the isotopic position unambiguously.

- (4) A compound is given the same name whether its labeled positions have been derived through carrier free or tracer level syntheses. The reasons for this are presented by Otvos and Wagner<sup>(3)</sup> and by Anderson<sup>(5)</sup>. The problem of how to name acetylene prepared from barium carbide- $C^{14}$  of either carrier-free or tracer levels of carbon- $^{14}$  activity is therefore resolved. These acetylenes are named "acetylene- $C_2^{14}$ ."
- (5) The simplest possible name consistent with good usage is always used. For example, the subscript "1" is never used to denote the presence in a compound of only one isotopic carbon atom and one position of labeling. In addition, when their use would add no clarity to the name, locants (numbers or Greek letters) are omitted. Thus, "methane- $C^{14}$ " and "acetylene- $C_2^{14}$ " are used in preference to "methane- $C_1^{14}$ " and "acetylene-1,2- $C_2^{14}$ ."
- (6) Parentheses are used when necessary to prevent ambiguity. Nomenclature rule 50<sup>(14)</sup> states "If it is necessary to avoid

---

(14) Austin M. Patterson, J. Am. Chem. Soc., 55, 3921 (1933).

---

ambiguity, the names of complex radicals will be placed in parentheses." Examples are the names "1-(2-furyl)propylamine" and "N-(2-furyl)propylamine." There are at least two classes of names for carbon-labeled compounds in which parentheses are useful:

- a. Names in which the position of labeling is doubtful to the reader because of uncertainty as to whether the isotope symbol precedes or follows the name or part of the name it modifies. (Patterson's discussion<sup>(11)</sup> with reference to the position of numbers has been mentioned in Part II of this paper). An example of such a name is "phenyl-1-C<sup>14</sup>-acetophenone." To many chemists this would indicate ring-labeling in the No. 1 position of the benzene nucleus attached to the  $\alpha$ -carbon atom of acetophenone. To others it might indicate labeling in the carbonyl-group of the compound. The present authors therefore call the ring-labeled structure "(phenyl-1-C<sup>14</sup>)-acetophenone," and the carbonyl-labeled structure "phenyl(aceto-1-C<sup>14</sup>)-phenone."
- b. One-word names, or one-word parts of names in which locants are not used. Consider, for example, the name "methylurea-C<sup>14</sup>." Does this name imply (1) carbonyl-labeled, (2) methyl-labeled, (3) both carbonyl- and methyl-labeled methylurea, or (4) methylurea of unknown labeling? The use of parentheses removes all doubt. Thus, the methyl-labeled compound is named "(methyl-C<sup>14</sup>)-urea," the carbonyl-labeled compound, "methyl(urea-C<sup>14</sup>)", and the doubly-labeled compound becomes "methylurea-C<sub>2</sub><sup>14</sup>." Similar examples are "9-fluorene(methanol-C<sup>14</sup>)" and "diphenyl(methane-C<sup>14</sup>)." Note that parentheses are not necessary in the names "ethyl-2-C<sup>14</sup>-urea," "ethyl carbamate-C<sup>14</sup>" and "ethyl-1-C<sup>14</sup>

carbamate." Note also that parentheses do not introduce, nor do away with the need for hyphens, in the names in which they are employed.

- (7) A compound known to contain isotopic carbon, but whose position or positions of labeling are unknown is designated in the name by preceding the isotope symbol with the lowercase letter "x." For example, glucose prepared photosynthetically in the presence of carbon- $C^{14}$  dioxide, would be named "glucose-x- $C^{14}$ " provided there was no knowledge of the position or positions of labeling. The small "x" is used in the chemical literature, and particularly in Beilstein, to denote positional uncertainty. The use of the question mark (?) in the place of "x" seems also to be justifiable, although the present authors do not recommend its use since it might connote uncertainty as to whether or not the molecule were labeled, or whether or not the proper isotope symbol had been employed.
- (8) Structures labeled with more than one isotope of carbon are named following the principle of "low numbers"<sup>(11)</sup>. Numbers referring to positions of labeling are given first precedence, while second precedence is given to the numbers indicating the atomic weight of the isotope. The following examples will illustrate the principle: "butane-1,2- $C^{14}$ -4- $C^{13}$ " and "butane-1- $C^{13}$ ,  $C^{14}$ " are preferred to "butane-1- $C^{13}$ -3,4- $C^{14}$ " and "butane- $C^{14}$ ,  $C^{13}$ ." Note, however, that  $ClC^{13}H_2CH_2C^{14}H_2C^{14}H_3$  is named "1-chloro-butane-1- $C^{13}$ -3,4- $C^{14}$ ."

- (9) Hyphens are placed between the locant (number or Greek letter) and the isotope symbol. The name "ethanol-1-C<sup>14</sup>" is therefore used rather than the name "ethanol-1C<sup>14</sup>." It might be argued that since no hyphen is used in the "extra" hydrogen designation<sup>(15)</sup>, it also

---

(15) Chem. and Eng. News, 27, 1303 (1949).

---

is unnecessary here. The present authors tentatively favor the use of the hyphen however, in names of compounds in which isotopes must be denoted since its inclusion would prevent ambiguity in names of compounds containing isotopes of oxygen and iodine. In the latter two instances the 0 and I symbols might be confused with the numbers zero and one. For example, the name "1,4-diiodopentane-1-I<sup>131</sup>" might seem preferable to "1,4-diiodopentane-1I<sup>131</sup>." Similarly, "1,4-pentanediol-1-O<sup>18</sup>" might seem preferable to "1,4-pentanediol-1O<sup>18</sup>." The question however, as to the use of the hyphen in this instance is one to be decided finally by the committee on Nomenclature, Spelling and Pronunciation of the American Chemical Society.

IV. Examples

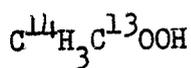
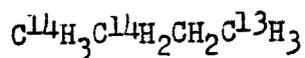
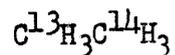
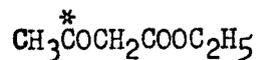
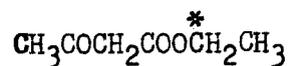
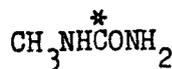
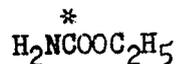
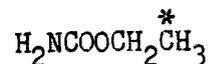
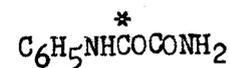
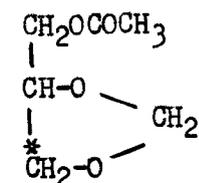
Following is a list of formulas with one or two names for each compound illustrating the principles set down in part III. For convenience, carbon-14 has been chosen as the isotopic carbon atom in compounds which are labeled with only one isotope, and its presence is indicated in the formula by the asterisk (\*).

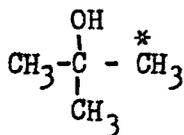
$^* \text{CH}_3\text{OH}$		methanol-C <sup>14</sup>
$\text{CH}_3^* \text{CH}_2\text{OH}$		ethanol-1-C <sup>14</sup> ethyl-1-C <sup>14</sup> alcohol
$^* \text{CH}_3^* \text{CH}_2\text{OH}$		ethanol-C <sub>2</sub> <sup>14</sup> ethyl-C <sub>2</sub> <sup>14</sup> alcohol
$\left\{ \begin{array}{l} \text{CH}_3^* \text{CH}_2\text{OH} \\ ^* \text{CH}_3 \text{CH}_2\text{OH} \end{array} \right\}$	mixture	ethanol-1,2-C <sub>1</sub> <sup>14</sup> ethyl-1,2-C <sub>1</sub> <sup>14</sup> alcohol
$\text{CH}_3^* \text{COOH}$		acetic-1-C <sup>14</sup> acid
$\text{CH}_3\text{COOCH}_2^* \text{CH}_3$		ethyl-2-C <sup>14</sup> acetate
$^* \text{CH}_3 \text{CN}$		acetonitrile-2-C <sup>14</sup> (16) methyl-C <sup>14</sup> cyanide

---

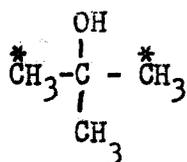
(16) This name is preferred to "(aceto-2-C<sup>14</sup>)-nitrile," since "acetonitrile" connotes only two carbon atoms, thus no possible ambiguity could exist by placing the isotope symbol at the end of the name.

---

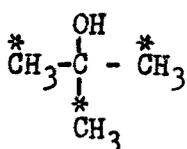
acetic-1-C<sup>13</sup>-2-C<sup>14</sup> acidbutane-1,2-C<sup>14</sup>-4-C<sup>13</sup>ethane-1-C<sup>13</sup>-2-C<sup>14</sup>ethyl (aceto-1-C<sup>14</sup>)-acetateethyl-1-C<sup>14</sup> acetoacetate(methyl-C<sup>14</sup>)-ureamethyl(urea-C<sup>14</sup>)ethyl carbamate-C<sup>14</sup>ethyl-2-C<sup>14</sup> carbamateoxamic-1-C<sup>14</sup> acidoxamide-1-C<sup>14</sup>oxamic-1-C<sup>14</sup> anilide1-ethyl 2-methyl oxalate-1-C<sup>14</sup>1-acetyl-2,3-methyleneglycerol-3-C<sup>14</sup>



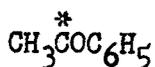
2-(methyl-C<sup>14</sup>)-2-propanol  
2-methyl-2-propanol-1-C<sup>14</sup>



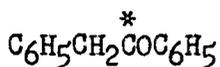
2-methyl-2-propanol-1,3-C<sup>14</sup>



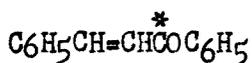
2-(methyl-C<sup>14</sup>)-2-propanol-1,3-C<sup>14</sup>  
tri(methyl-C<sup>14</sup>)-carbinol



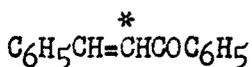
(aceto-1-C<sup>14</sup>)-phenone



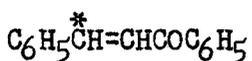
$\alpha$ -phenyl(aceto-1-C<sup>14</sup>)-phenone  
benzyl phenyl ketone-C<sup>14</sup>



$\alpha$ -benzylidene(aceto-1-C<sup>14</sup>)-phenone  
phenyl styryl ketone-C<sup>14</sup>



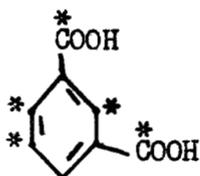
$\alpha$ -benzylidene(aceto-2-C<sup>14</sup>)-phenone  
 $\alpha$ -benzylidene(aceto- $\alpha$ -C<sup>14</sup>)-phenone  
phenyl styryl- $\beta$ -C<sup>14</sup> ketone



$\alpha$ -(benzylidene- $\alpha$ -C<sup>14</sup>)-acetophenone  
phenyl styryl- $\alpha$ -C<sup>14</sup> ketone



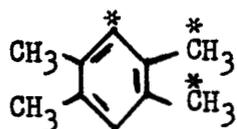
benzene-1,3,4-C<sup>14</sup>-carboxylic-C<sup>14</sup>  
acid



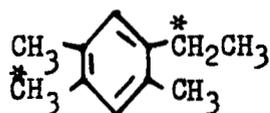
1,3-(benzene-2,4,5-C<sub>3</sub><sup>14</sup>)-  
di(carboxylic-C<sup>14</sup>) acid



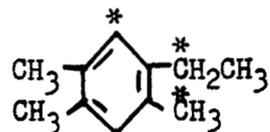
durene- $\alpha^1, \alpha^4$ -C<sub>2</sub><sup>14</sup>



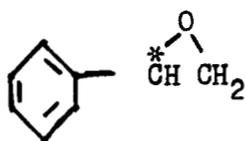
durene- $\alpha^1, \alpha^2, 3$ -C<sub>3</sub><sup>14</sup>



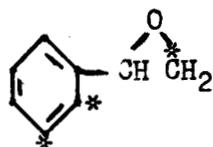
1-methyl-C<sup>14</sup>-4-(ethyl-1-C<sup>14</sup>)-  
2,5-dimethylbenzene



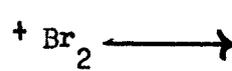
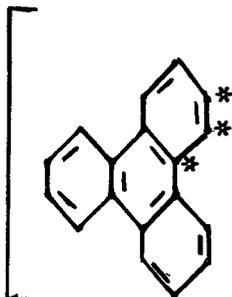
1-methyl-C<sup>14</sup>-2-(ethyl-1-C<sup>14</sup>)-  
4,5-dimethylbenzene-3-C<sup>14</sup>



styrene- $\alpha$ -C<sup>14</sup> oxide



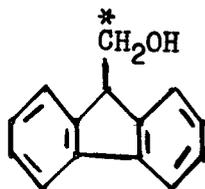
styrene-2,3, $\beta$ -C<sub>3</sub><sup>14</sup> oxide



monobromotriphenylene substituted  
in the 2-position

2(3,6,7,10,11)-monobromotri-  
phenylene-3,4,4a-C<sup>14</sup><sub>3</sub>

2(or 3,6,7,10,11)-monobromotri-  
phenylene-3,4,4a-C<sup>14</sup><sub>3</sub>



9-fluorene(methanol-C<sup>14</sup>)  
9-fluorenyl(carbinol-C<sup>14</sup>)