

- (4) *Ibid.*, p 44.
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APPENDICES (Available on request)

1. Data base: list of 308 journal articles cited
2. Cumulation/computation of data; histograms
 - 2.1 Citations, cumulations tables/histograms
 - 2.2 Sum of Citation Ages per Source Article, computations/histograms
 - 2.3 Average Age/percentage of citation computations/histograms
3. Chi-square test computations

Revised Nomenclature for Highly Fluorinated Organic Compounds

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The system described herein has been adopted by the American Chemical Society as authorized nomenclature for highly fluorinated organic compounds. Its main features are the introduction of the symbol "F" to convey the sense of "perfluoro" and the prefix "hydryl" to describe solitary hydrogen atoms in an almost completely fluorinated structure, with codification of standard usage for these prefixes.

There has been no change in authorized nomenclature for organic fluorine compounds since 1952, when the conventions "H" and "perhalo" were adopted.¹ Prior to that time, it had been necessary to name and locate each fluorine atom in a molecule such as $\text{H}(\text{CF}_2)_5\text{CF}_3$. The "H" convention simplified and shortened nomenclature in this and similar cases but unfortunately could not be used together with "perfluoro," so that, for example, $\text{H}(\text{CF}_2)_6\text{Cl}$ remained 6H-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorochlorohexane. Moreover, the term "perfluoro" was employed erroneously and ambiguously in spite of its wide usage, since it sometimes included a functional group and at other times did not; for example, both $(\text{CF}_3)_2\text{NH}$ and $(\text{CF}_3)_2\text{NF}$ were referred to in the literature as perfluorodimethylamine. The new system replaces "perfluoro" with "F", which conveys the same sense of complete fluorination without the use of locants, and replaces "H" with "hydryl," a collective prefix which can be applied in conjunction with "F" to functional compounds.

Established systems of organic chemical nomenclature are all based on the prevalence of hydrogen. The total number of hydrogen atoms in a molecule is not stated but must be found by satisfying all the conditions stipulated in the name concerning atomic identity, valence state, and structure. Any atom whose identity is neither stated nor implied in any part of the name is assumed to be a hydro-

gen atom. The main principle of the rules presented here is the transfer of this assumed prevalence from hydrogen to fluorine, by use of the symbol "F". When this symbol is used, any atom attached to carbon whose identity is neither specifically stated nor implied in any part of the name is assumed to be a fluorine atom. As the parent "F" compound or radical, by this definition, contains no hydrogen atoms attached to carbon atoms in the named backbone, any such hydrogen atoms actually present cannot be regarded as residual but must be named as substituents, and the total number of fluorine atoms is not stated but results from satisfying all the stipulated conditions of atomic identity, valence state, and structure. In other words, substituent atoms or groups are regarded as having been substituted for fluorine, not for hydrogen.

These rules are concerned with what is tacit within a name, that is, the nature of unspecified atoms, rather than with structural features. Consequently, once the implication of the symbol "F" is made, all other features of the molecule can be described, in general, by conventional naming practices.

The rules deal with three areas: (a) definition of the symbol "F" and delineation of its proper usage, (b) treatment of fluorocarbon derivatives containing heteroatoms, and (c) designation of hydrogen atoms where only a few of these are present. The present rules deal only with compounds

containing a recognizably "organic" structure; the nomenclature of highly fluorinated inorganic structures is now under active study by another group.†

1. Applicability

These rules are intended for use when the following conditions are satisfied:

1.1 The parent compound or radical in question is named in accordance with approved rules of systematic organic nomenclature, or by a trivial name accepted by the IUPAC (see *J. Amer. Chem. Soc.*, **82**, 5545 (1960); *Pure Appl. Chem.*, **11**, 1-260 (1966); or IUPAC Nomenclature of Organic Chemistry, Sections A, B, C, Butterworths, London, 1971). These rules should not be applied to trade names or to trivial names unaccepted by the IUPAC.

1.2 The proportion of fluorine atoms attached to atoms comprising the parent compound or radical is large enough to make application of the rules advantageous.

2. Symbols and Terms

2.1 The prefix "fluoro" is retained in its accepted sense, denoting substitution of hydrogen by fluorine.

2.2 The prefix "perfluoro" is not used.

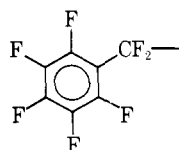
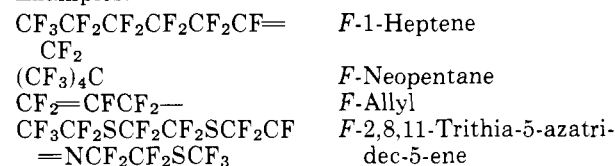
2.3 The symbol "*F*" (italic, capitalized) replaces the term "perfluoro." Application of this symbol is discussed in section 3. In speech, "*F*" is pronounced "eff," not "perfluoro."

2.4 The prefix "hydriyl" denotes substitution of fluorine by hydrogen. Application of this term is discussed in section 5.

3. Significance of the Symbol "*F*"

3.1 The symbol "*F*" prefixed to the name of a parent compound or radical signifies replacement of all hydrogen atoms attached to carbon atoms in that parent compound or radical, except as specified in Rule 3.2. Hydrogen atoms attached to carbon atoms that are part of carbon-carbon unsaturation or carbon-nitrogen unsaturation are not excepted and are included in the substitution signified by "*F*".

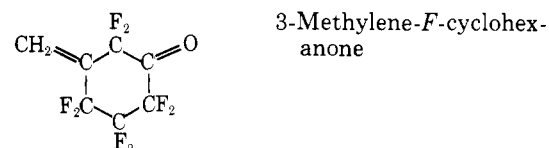
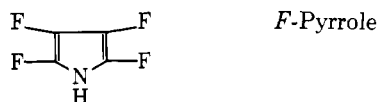
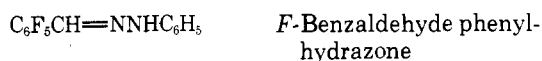
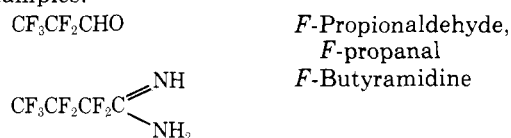
Examples:



F-Benzyl

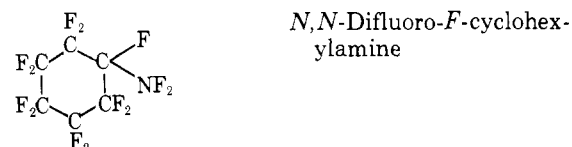
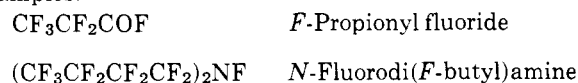
3.2 The symbol "*F*" does *not* denote replacement by fluorine of hydrogen atoms that are attached to atoms other than carbon or are integral parts of recognized functional groups such as aldehydes, acids, amides, oximes, amines, etc.

Examples:



3.3 If any fluorine atoms are attached to atoms other than carbon, or are incorporated in functional groups, such fluorine atoms must be specifically designated.

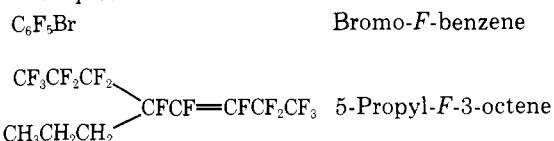
Examples:



4. Placement of the Symbol "*F*"

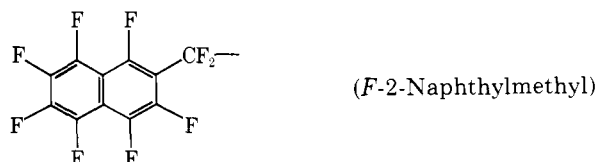
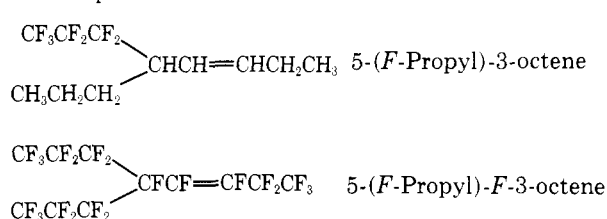
4.1 The symbol "*F*" immediately precedes the name of the parent compound or radical that it modifies.

Examples:



4.2 When radicals are thus modified in one-word names, parentheses should be used.

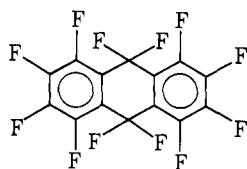
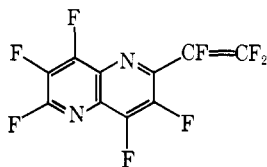
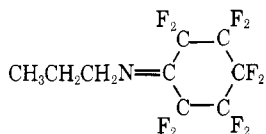
Examples:



4.3 Nonseparable prefixes, whether operational (aza, dehydro, cyclo, deoxy, homo, hydro, nor, etc.) or structural (iso, threo, trans, para, etc.) are an integral part of the name of the parent compound or radical.

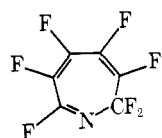
†Inquiries should be addressed to Dr. Kurt L. Loening, Chemical Abstracts Services, Ohio State University, Columbus Ohio 43210.

Examples:

*F*-9,10-Dihydroanthracene2-(*F*-Vinyl)-*F*-1,5-diazanaphthalene*N*-(*F*-Cyclohexylidene)-propylamine

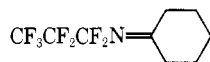
4.4 Similarly, the symbol “*H*”, representing “indicated” hydrogen, is an integral part of the name of the parent compound or radical.

Examples:

*F*-2*H*-Azepine

4.5 On the other hand, substitutive prefixes (chloro, hydryl, amino, nitro, etc.) are separable and are placed *before* the symbol “*F*” (see also Rules 4.1 and 4.2).

Examples:

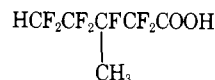
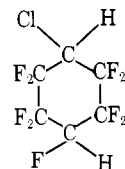
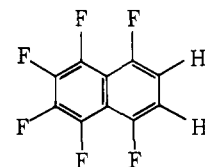
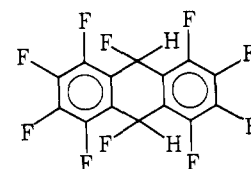
Nitro-*F*-benzene*N*-Cyclohexylidene-*F*-propylamine

5. Naming Hydrogen Attached to Carbon

When the symbol “*F*” is used, any hydrogen atoms attached to carbon atoms in the parent compound or radi-

cal are regarded as substitutive and must be specifically designated. Designation is accomplished by use of the substitutive prefix “hydryl.”

Examples:

1,1,5-Trihydryl-*F*-1-pentanol5-Hydryl-3-methyl-*F*-pentanoic acid1-Chloro-1,4-dihydryl-*F*-cyclohexane2,3-Dihydryl-*F*-naphthalene9,10-Dihydryl-*F*-9,10-dihydroanthracene

ACKNOWLEDGMENT

The author is indebted to the following members of the nomenclature committee of the Division of Fluorine Chemistry for their cooperation and contributions: Dr. Henry C. Brown, Dr. Alan F. Clifford, Dr. George H. Crawford, Dr. Murray Hauptschein, Dr. Douglas A. Rausch, and Dr. F. W. Swamer. The nomenclature committee of the American Chemical Society, under the chairmanship of Dr. Kurt L. Loening, has been most helpful in critically reviewing all the successive versions in the evolution of these revisions.

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Vapor Pressure Data in Recent Handbook Unreliable

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The Clausius-Clapeyron equation

$$\frac{dP}{dT} = \frac{\Delta H}{T\Delta V} \quad (1)$$

treats the general case of the thermodynamically reversible transformation of matter from one phase to another at an equilibrium pressure, *P*, and an absolute temperature *T*. ΔH is the net enthalpy change, and ΔV is the net volume change associated with the transformation. By adopting

three assumptions—(i) that the volume of the condensed phase may be neglected in comparison with that of the vapor, (ii) that the vapor phase behaves like a perfect gas, and (iii) that the enthalpy change is constant for the range of temperature under consideration—eq 1 can be converted to the form

$$\log P = \frac{-\Delta H}{2.303RT} + B = \frac{-0.2185\Delta H}{T} + B \quad (2)$$