Nomenclature of alcohols and simple esters[1]

HENRY RAKOFF, Northern Regional Research Laboratory[2],
Peoria, Illinois 61604

INTRODUCTION

The AOCS Subcommittee on Nomenclature has undertaken the task of defining nomenclature as related to the chemistry of fats and oils. A general paper on nomenclature (1), as well as one on the nomenclature of carboxylic acids (2) already has appeared. A paper on acylglycerols (glycerides) (3) is appearing in this issue, as well as a paper on nitrogen compounds (4). In continuing this work and in keeping with the criteria outlined in ref. 1, most of the names recommended are used in *Chemical Abstracts* and are recommended by the Committee on Nomenclature, Division of Organic Chemistry, American Chemical Society (5,6).

NOMENCLATURE OF ALCOHOLS

Alcohols are compounds that contain a hydroxy group (OH) attached to an aliphatic carbon. Unsubstituted alcohols are named by dropping the terminal letter "e" from the name of the parent hydrocarbon and adding the suffix "ol." The position of the OH group is indicated by a location number.

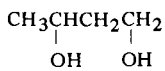
$CH_3CHOHCH_3$ 2-Propanol

$CH_3CH_2CH(CH_3)CHOHCH_3$ 3-Methyl-2-pentanol

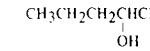
 Cyclohexanol

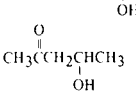
The names isopropanol, *sec*-butanol, and *tert*-butanol are incorrect, because there are no hydrocarbons designated isopropane, *sec*-butane, or *tert*-butane to which the suffix "ol" can be added.

Diols not containing other functional groups are named by adding the suffix "diol" to the name of the parent hydrocarbon without elision of the final "e." The positions of the OH groups are indicated by location numbers, and the chain is numbered so as to give the lowest possible numbers to the OH groups.

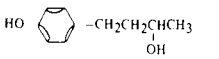
 1,3-Butanediol

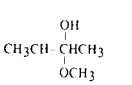
In substituted alcohols, where the alcohol is not the principal functional group, the presence of the OH group is indicated by the prefix "hydroxy." Some common groups that take precedence over alcohol groups are carboxylic acid, acid halide, amide, aldehyde, nitrile, and ketone. Some examples of naming such "mixed compounds" are given below.

 3-Hydroxyhexanoic acid

 4-Hydroxy-2-pentanone

Some common groups that follow alcohol in order of precedence are phenol, amine, and ether. Examples for naming such compounds appear below.

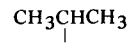
 4-(*p*-Hydroxyphenyl)-2-butanol

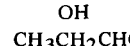
 3-Methoxy-2-butanol

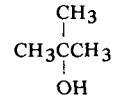
Radicofunctional names of alcohols consist of the radical name derived from the parent compound followed by the word "alcohol."

CH_3CH_2OH Ethyl alcohol

$CH_3CH_2CH_2CH_2CH_2OH$ Pentyl alcohol

 Isopropyl alcohol

 *sec*-Butyl alcohol

 *tert*-Butyl alcohol

Recommended and other acceptable names for saturated, unsaturated, and miscellaneous alcohols appear in Tables I, II, and III.

NOMENCLATURE OF CARBOXYLIC ESTERS

The naming of carboxylic esters follows closely that of carboxylic acids (2). An ester is designated by citing the radical name of the alcohol and then, as a separate word, the name of the acid modified as discussed in the following paragraphs.

If the acid is named by the "oic acid" system, the ester is named by converting "ic acid" to "ate."

TABLE I

Saturated Alcohols[a]

Formula	Recommended names	Other acceptable names
CH_3OH	†*Methanol	
CH_3CH_2OH	*Ethyl alcohol	†Ethanol
$CH_3CH_2CH_2OH$	*Propyl alcohol	†Propanol
$CH_3CHOHCH_3$	*Isopropyl alcohol	†2-Propanol (not isopropanol)
$CH_3CH_2CH_2CH_2OH$	*Butyl alcohol	†Butanol
$CH_3CH_2CHOHCH_3$	**sec*-Butyl alcohol	†2-Butanol (not *sec*-butanol)
CH_3CHCH_2OH (CH₃ branch)	*Isobutyl alcohol	2-Methylpropanol
$(CH_3)_3COH$	**tert*-Butyl alcohol	2-Methyl-2-propanol (not *tert*-butanol)
$CH_3(CH_2)_3CH_2OH$	*Pentyl alcohol	†Pentanol
$(CH_3)_2CHCH_2CH_2OH$	*Isopentyl alcohol	3-Methylbutanol
$CH_3(CH_2)_4CH_2OH$	*Hexyl alcohol	†Hexanol
$(CH_3)_2CHCH_2CH_2CH_2OH$	*Isohexyl alcohol	4-Methylpentanol
$CH_3(CH_2)_5CH_2OH$	*Heptyl alcohol	†Heptanol
$CH_3(CH_2)_6CH_2OH$	*Octyl alcohol	†Octanol
$CH_3(CH_2)_7CH_2OH$	*Nonyl alcohol	†Nonanol
$CH_3(CH_2)_8CH_2OH$	*Decyl alcohol	†Decanol
$CH_3(CH_2)_9CH_2OH$	*Undecyl alcohol	†Undecanol
$CH_3(CH_2)_{10}CH_2OH$	*Dodecyl alcohol	†Dodecanol, lauryl alcohol
$CH_3(CH_2)_{11}CH_2OH$	†*Tridecanol	Tridecyl alcohol
$CH_3(CH_2)_{12}CH_2OH$	†*Tetradecanol	Myristyl alcohol, tetradecyl alcohol
$CH_3(CH_2)_{13}CH_2OH$	†*Pentadecanol	Pentadecyl alcohol
$CH_3(CH_2)_{14}CH_2OH$	†*Hexadecanol	Palmityl alcohol, hexadecyl alcohol
$CH_3(CH_2)_{15}CH_2OH$	†*Heptadecanol	Heptadecyl alcohol
$CH_3(CH_2)_{16}CH_2OH$	†*Octadecanol	Stearyl alcohol, octadecyl alcohol

[a]Names used by *Chemical Abstracts* for the unsubstituted alcohol only are marked with an asterisk (*); for the substituted alcohol only, with a dagger (†); and for both substituted and unsubstituted alcohol, with both an asterisk and a dagger.

[1]This paper is a part of the nomenclature program of the AOCS Nomenclature Subcommittee.

[2]ARS, USDA.

TABLE II

Unsaturated Alcohols[a,b]

Formula	Recommended names	Other acceptable names
$CH_2=CHCH_2OH$	*Allyl alcohol	†Propenol
$CH_3CH=CHCH_2OH$	†*2-Butenol	Crotonyl alcohol
$CH_3CH_2CH=CH(CH_2)_7CH_2OH$	†*(Z)-9-Dodecenol	Lauroleyl alcohol
$CH_3(CH_2)_3CH=CH(CH_2)_7CH_2OH$	†*(Z)-9-Tetradecenol	Myristoleyl alcohol
$CH_3(CH_2)_5CH=CH(CH_2)_7CH_2OH$	†*(Z)-9-Hexadecenol	Palmitoleyl alcohol
$CH_3(CH_2)_{10}CH=CH(CH_2)_4CH_2OH$(*cis*)	†*(Z)-6-Octadecenol	Petroselinyl alcohol
$CH_3(CH_2)_{10}CH=CH(CH_2)_4CH_2OH$(*trans*)	†*(E)-6-Octadecenol	Petroselaidyl alcohol
$CH_3(CH_2)_7CH=CH(CH_2)_7CH_2OH$(*cis*)	†*(Z)-9-Octadecenol	Oleyl alcohol
$CH_3(CH_2)_7CH=CH(CH_2)_7CH_2OH$(*trans*)	†*(E)-9-Octadecenol	Elaidyl alcohol
$CH_3(CH_2)_4(CH=CHCH_2)_2(CH_2)_6CH_2OH$	†*(9Z,12Z)-9,12-Octadecadienol	Linoleyl alcohol
$CH_3CH_2(CH=CHCH_2)_3(CH_2)_6CH_2OH$	†*(9Z,12Z,15Z)-9,12,15-Octadecatrienol	Linolenyl alcohol
$CH_3(CH_2)_7C=C(CH_2)_7CH_2OH$	†*9-Octadecynol	Stearolyl alcohol

[a]Names used by *Chemical Abstracts* for the unsubstituted alcohol only are marked with an asterisk (*); for the substituted alcohol only, with a dagger (†); and for both substituted and unsubstituted alcohol, with both an asterisk and a dagger.

[b]For the Z and E system for designating configuration about a carbon-carbon double bond, see refs. 7-9.

TABLE III

Miscellaneous Alcohols[a]

Formula	Recommended names	Other acceptable names
$C_6H_5CH_2OH$	†*Benzyl alcohol	
$C_6H_5CH_2CH_2OH$	†*Phenethyl alcohol	2-Phenylethanol
CH_2OHCH_2OH	*Ethylene glycol	†1,2-Ethanediol
$CH_3CHOHCH_2OH$	†*1,2-Propanediol	Propylene glycol
$CH_2OHCH_2CH_2OH$	†*1,3-Propanediol	Trimethylene glycol
$CH_2OHCHOHCH_2OH$	*Glycerol	†1,2,3-Propanetriol
$C(CH_2OH)_4$	†*Pentaerythritol	2,2-bis(Hydroxymethyl)-1,3-propanediol
$(C_6H_5)_3COH$	†*Triphenylmethanol	Trityl alcohol

[a]Names used by *Chemical Abstracts* for the unsubstituted alcohol only are marked with an asterisk (*); for the substituted alcohol only, with a dagger (†); and for both substituted and unsubstituted alcohol, with both an asterisk and a dagger.

$CH_3(CH_2)_3COOCH_2CH_3$ Ethyl pentanoate
$CH_3CH_2CH_2CH=CHCH_2COOCH_3$ Methyl 3-heptenoate
$CH_3OOC(CH_2)_4COOCH_3$ Dimethyl hexanedioate

Substituents on the alcohol or acid portions of the ester, or both, are indicated by a prefix and a location number. Numbering on the acid starts with the carboxyl carbon and on the alcohol with the carbon attached to the oxygen.

$CH_3CHCH_2COOCH_2CH_2CH_3$ (OH) Propyl 3-hydroxybutanoate
$CH_3CH_2CH_2COOCH_2CH_2CH_2OH$ (O) 3-Hydroxypropyl butanoate
$CH_3CCH_2COOCH_2CHCH_2CH_3$ (O; OH) 2-Hydroxybutyl 3-oxobutanoate

If the acid is named by the "carboxylic acid" system, the ester is designated by citing the radical name of the alcohol and then the name of the acid with the "ic acid" changed to "ate." For example, the methyl ester of cyclohexanecarboxylic acid would become methyl cyclohexanecarboxylate.

In the "trivial system," used only for acids of long standing and wide usage, the ester is designated by citing the radical name of the alcohol followed by the name of the acid with the "ic acid" changed to "ate."

$CH_3(CH_2)_{16}COOCH_3$ Methyl stearate
$CH_3(CH_2)_7CH=CH(CH_2)_7COOCH_2CH_3$ Ethyl oleate
$C_2H_5OOC(CH_2)_3COOC_2H_5$ Diethyl glutarate

REFERENCES

1. Goheen, G.E., JAOCS 45:388a (1968).
2. Dupuy, H.P., Ibid. 45:390A (1968).
3. Jensen, R.C., Ibid. 52:62A (1975).
4. Meisters, G.J., Ibid. 52:67A (1975).
5. "The Naming and Indexing of Chemical Compounds from Chemical Abstracts," Chem. Abstr. 56 (1962) and subsequent annual subject indexes.
6. Fletcher, J.H., O.C. Dermer, and R.B. Fox, Advan. Chem. Ser. 126 (1974).
7. International Union of Pure and Applied Chemistry, J. Org. Chem. 35:2851 (1970).
8. Blackwood, J.E., C.L. Gladys, K.L. Loening, A.E. Petrarca, and J.E. Rush, J. Amer. Chem. Soc. 90:509 (1968).
9. Blackwood, J.E., C.L. Gladys, A.E. Petrarca, W.H. Powell, and J.E. Rush, J. Chem. Soc. 8:30 (1968).

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Barker named SCC director

AOCS member Graham Barker has been named director of Area I of The Society of Cosmetic Chemists. Barker was installed as director at the society's Annual Scientific Meeting in December in New York City. ■

Liquid densities discussed in new publication

Liquid Densities of Oxygen, Nitrogen, Argon, and Parahydrogen recently has been published by the National Bureau of Standards. Authored by H.M. Roder, the book contains tables of pressure, volume, density, and temperature for saturated liquid and for compressed liquid states from the triple point to the critical point of oxygen, nitrogen, argon, and parahydrogen. The table entries of temperature are in Kelvin and degrees Celsius; table entries in pressure are in bars and kp/cm^2. Volumes or densities are given in several different units, and density ratios are tabulated for each entry. Estimates of the uncertainty for the tabulated data are given. ■