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Rules of Carbohydrate Nomenclature

This report is the result of a cooperative effort by the Nomenclature Committee of the Division of Carbohydrate Chemistry of the American Chemical Society, under the chairmanship of Dr. M. L. Wolfrom, and a British Committee on Carbohydrate Nomenclature [a Subcommittee of the Publications Committee of The Chemical Society (London)]. The report was approved by the Committee on Nomenclature, Spelling, and Pronunciation of the American Chemical Society and by the Council of the American Chemical Society in March, 1962, on a tentative basis for at least one year.

Use may dictate some revisions in these rules. Any official changes that may arise will be reported at the beginning of the "Additions and Corrections" Section, which appears in each December issue of this Journal.

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The Rules of Carbohydrate Nomenclature, which follow, have been devised primarily for the English language. It is to be understood that minor alterations, especially in regard to word endings, may be desirable in adapting the rules to other languages. The rules are recommended for use whenever systematic names for carbohydrates and their derivatives are required.

Rule 1.—Carbohydrate nomenclature should follow the general principles of established organic nomenclature.

Rule 2.—As few changes as possible will be made in terminology universally adopted.

COMMENT.—This principle is stated in the Introduction to the International Union of Pure and Applied Chemistry Rules of Organic Nomenclature as published in "Nomenclature of Organic Chemistry, 1957" (Butterworths Scientific Publications); J. Am. Chem. Soc., 82, 5545 (1960); Chem. Soc. (London), Spec. Publ., No. 14, 48 (1960).

Rule 3.—The names "aldose" or "ketose" will be used in a generic sense to denote the respective character of the reducing, or potentially reducing, group of the monosaccharide or derivative thereof. In an aldose, the carbon atom of the aldehyde function is atom number one; and, in a ketose, the carbonyl carbon atom has the lower possible number.

For indicating the number of carbon atoms in the normal chain, the appropriate one of the following names will be used: triose, tetrose, pentose, hexose, heptose, octose, nonose, etc.

Rule 4.—Configurational relationships will be denoted by the capital letter prefixes D and L, which in print will be small capital Roman letters and which are pronounced "dee" and "ell" (not "dextro" and "levo"). Such symbols will be placed immediately before the sugar stem name and be employed only with compounds which have been definitively related to the reference-standard glyceraldehyde (see Rule 5). In a definitive name, the configurational symbol shall not be omitted.

If the optical rotational sign under specified conditions is to be indicated, this may be done by adding (dextro) or (levo), which are italicized in print, or by adding (+) or (-). Racemic modifications may be indicated by the prefixes DL, or (\pm) . With certain isomers, it may be desirable to employ the prefix *meso*; see examples in Rules 23 and 24.

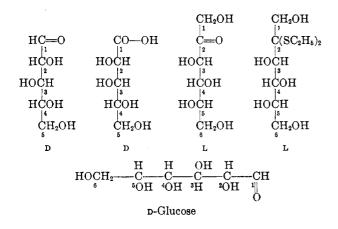
Examples:

D-Glucose or D-(dextro)-glucose or D-(+)-glucose D-Fructose or D-(levo)-fructose or D-(-)-fructose DL-Glucose or (\pm) -glucose

Rule 5.—Carbohydrates having the same configuration of the highest numbered asymmetric carbon atom (but see Rule 22) as that of D-(dextro)-glyceraldehyde will belong to the D-configurational series; those having the opposite configuration will belong to the L series. The absolute configuration of D-(dextro)-glyceraldehyde is:



COMMENT.—For the conventions employed in the two-dimensional representations of carbohydrate configurations, see *Chem. Eng. News*, **26**, 1623 (1948). When more than one configurational center is involved, the formulas may be written horizontally, in which case the top orienting group (carbon one) lies to the extreme right and the Fischer conventions are thus altered. In making a configurational interpretation of formulas so written, it is necessary to rotate the plane of depiction so that carbon atom one is at the top.



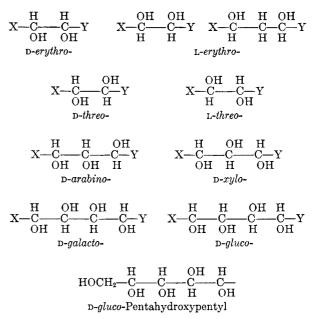
Rule 6.—The configuration of a group of consecutive but not necessarily contiguous asymmetric carbon atoms (such as >CHOH, >CHOCH₃, >CHOAc, or >CHNH₂), containing one to four asymmetric carbon atoms, will be designated by the appropriate one of these prefixes:

Asymmetric Carbons	Prefixes
one	glycero
\mathbf{two}	erythro, threo
\mathbf{three}	arabino, lyxo, ribo, xylo
four	allo, altro, galacto, gluco, gulo, ido, manno, talo

Each is D or L, as D-talo or L-manno. The prefix, which is derived by omitting the last two letters from the name of the aldose having the same configuration as the group to which it refers, is to be uncapitalized, and will be italicized in print. It is inserted into the name as the final step, and immediately precedes the prefix denoting the number of carbon atoms in the chain. Examples:

In each formula below, the principal function is at Y.

$$\begin{array}{c} H & OH \\ X - \begin{matrix} C - Y \\ OH \end{matrix} & \begin{matrix} X - \begin{matrix} C - -Y \\ H \end{matrix} \\ D - glycero - \end{matrix} \\ L - glycero - \end{matrix}$$



Rule 7.—Ketoses having the carbonyl group at carbon atom number two will be named by means of the suffix "-ulose"; before this will be a prefix denoting the number of carbon atoms in the chain, which, in turn, will be preceded by the prefix denoting the configuration of the group of asymmetric centers present (see Rule 6).

Ketoses having the carbonyl group at a carbon atom other than number two will be named by inserting the appropriate position-numeral immediately before the prefix denoting the number of carbon atoms in the chain.

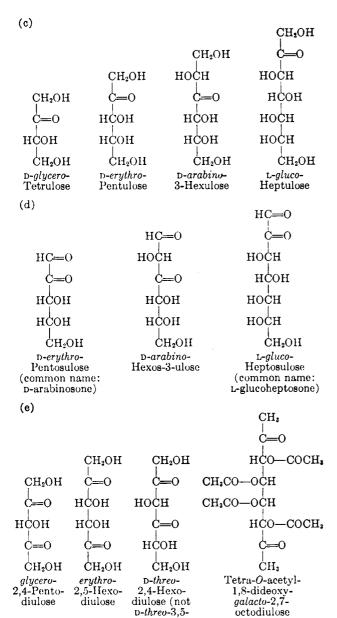
A sugar which is *both an aldose and a ketose* will be named by replacing the final "e" in the name of the (formally) parent aldose by the suffix "-ulose," preceded by the appropriate position-numeral, and then adding the appropriate configurational prefixes.

Ketoses having two ketonic carbonyl groups will be named by means of the suffix "-diulose"; before this will be placed a prefix denoting the number of carbon atoms in the chain, which, in turn, will be preceded by the numerals designating the positions of the carbonyl groups and the prefix denoting the configuration of the group of asymmetric centers present (see Rule 6).

Examples:

- (a) Permissible trivial names established by usage:
 - D-Fructose for D-arabino-hexulose
 - D-Psicose for D-ribo-hexulose
 - p-Sorbose for p-xylo-hexulose
 - D-Tagatose for $D-\bar{l}yxo$ -hexulose and the corresponding names for the L forms; sedoheptulose for D-altro-heptulose
 -) Names that cannot be used as definitive names, because they have incorrect structural implications:
 - Glycerulose (for 1,3-dihydroxy-2-propanone)
 - D-Erythrulose or D-threulose (for D-glycero-tetrulose)
 - D-Arabinulose or D-ribulose (for D-erythro-pentulose)
 - p-Lyxulose or p-xylulose (for p-threo-pentulose) and the corresponding names for the L forms

2-Deoxy-L-xylo-hexose

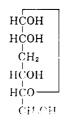


Rule 8.—When an alcoholic hydroxyl group of a monosaccharide is replaced by a hydrogen atom, the compound will be named by attaching by a hyphen, before the sugar name, the appropriate numeral (indicating position), a hyphen, and the prefix "deoxy." The configuration of the sugar will be designated, when necessary, as given in Rule 6.

Hexodiulose)

COMMENT.—Trivial names, established by usage, include: D-fucose (6-deoxy-D-galactose) and L-rhamnose (6-deoxy-L-mannose).

Examples:



3 - Deoxy - α - D - ribo - hexopyranose (see rules 15 and 18)
 2-Deoxy-D-erythro-pentose (2-deoxy-D-arabinose or, as commonly termed, 2-deoxy-D-ribose; both incorrect)

4-Deoxy- α -D-glycero-pentulofuranose (see Rules 15 and 18)

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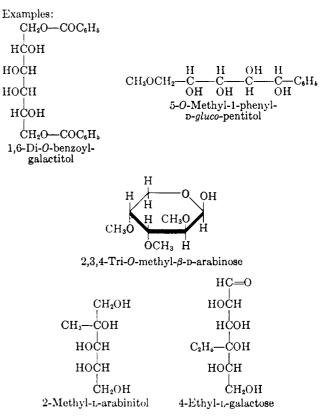
6-Deoxy-1,2-O-isopropylidene-β-L-idofuranose				
2,6-Dideoxy-3-O-methyl-B-D-lyxo-hexo	pyranose			
2-Amino-2-deoxy-α-D-galactopyranose	(common	name:	D-	
galactosamine)				
2-Amino-2-deoxy-a-D-glucopyranose	(common	name:	D•	
glucosamine)				
2-Acetamido-2-deoxy-α-D-glucopyrance	se			
2-Chloro-2-deoxy-α-D-glucopyranose				

. . .

6-Deoxy-6-iodo- α -D-galactopyranose

Rule 9.—When the hydrogen atom of an alcoholic hydroxyl group of a carbohydrate is replaced, an italic capital letter O (for oxygen) will be attached by a hyphen directly before the replacement prefix. The Oprefix need not be repeated for multiple replacements by one kind of group. Similar principles apply to replacement on nitrogen and sulfur (prefixes, N, S).

(The prefix C may be used to indicate replacement on carbon, to avoid possible ambiguity.)



2-Deoxy-2-(N-methylacetamido)- α -L-glucopyranose 3,4-Di-C-methyl-2-O-methyl- α -D-glucofuranose

Rule 10.—When the hydrogen atom of an alcoholic hydroxyl group of a carbohydrate (see Rule 9) is replaced by another atom or group, the name of the parent compound may be retained as the root for the substituted compound. In such names, the prefix (denoting the substituent) will be attached directly to the root and not be spaced from it.

COMMENT.—See Rule 16. Examples:

Rule 11.—An ester formed from a sugar or sugar derivative by reaction with one or more of its alcoholic hydroxyl groups may be named by placing, after the sugar name and separated therefrom by a space, the

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appropriate numeral (indicating position) and a hyphen, as prefix to the name of the group derived from an acid.

Examples:

 α -D-Glucopyranose 3-acetate

Methyl β -D-talofuranoside 2-benzoate

COMMENT.—Naming of O-acyl derivatives of carbohydrates may follow this terminology or Rule 9.

Examples:

- (a) Esters of monobasic carboxylic acids
 - (1) α -D-glucopyranose pentaacetate; penta-O-acetyl- α -Dglucopyranose
 - (2) β -L-Mannopyranuronic acid 2-benzoate; 2-O-benzoyl- β -L-mannopyranuronic acid
- (3) 2-Acetamidotetra-O-acetyl-2-deoxy-D-glucopyranose (b) Esters of sulfonic acids
- (1) Methyl β -D-galactoside 2,3,4-triacetate 6-methanesulfonate; methyl 2,3,4-tri-O-acetyl-6-O-(methylsulfonyl)-β-Dgalactoside
- (2) Methyl α -D-glucopyranoside 6-p-toluenesulfonate; methyl 6-O-(p-tolylsulfonyl)- α -p-glucopyranoside
- (c) Esters of nitric acid
 - (1) Methyl β -D-galactopyranoside 6-nitrate; methyl 6-Onitro- β -D-galactopyranoside
 - (2) D-Mannitol 1,6-dinitrate; 1,6-di-O-nitro-D-mannitol
 - (3) Methyl 4,6-O-ethylidene- β -D-glucoside 2,3-dinitrate; methyl 4,6-O-ethylidene-2,3-di-O-nitro-B-D-glucoside
- (d) Esters of polybasic acids are usually named by Rule 11 (see Rule 25)
 - (1) β -D-Glucopyranose 6-(dihydrogen phosphate)
 - α -D-Glucofuranose 6-(disodium phosphate) (2)
 - (3) α -D-Glucopyranose 6-(benzyl hydrogen phosphate)
 - (4) α -D-Glucopyranose 6-(benzyl methyl phosphate)

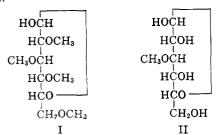
Rule 12.—Class terms (excepting amine) such as acetal, alcohol, anhydride, ether, glycoside, ketone, sulfide, xyloside, and the like, which, when used singly, represent no definite unsubstituted compound, are used as separate words.

Examples:

 β -D-Idose 2,3,4,6-tetramethyl ether Methyl α -D-mannopyranoside Ethyl β -L-xylofuranoside Di-D-fructopyranose 1,2':2,1'-dianhydride (see Rule 34)

Rule 13.—When ethers of polyhydric alcohols, or derivatives thereof, are named as ethers, the name of the parent alcohol will be the first word, "ether" the last word, and the name of the appropriate radical (or radicals) will be the middle word (or words).

COMMENT.—The term "ether" does not apply to compounds derived by substitution of the hydrogen atom of the hemiacetal hydroxyl group of the reducing or glycosidic carbon atom. Examples:



I. β -D-Glucose 2,3,4,6-tetramethyl ether, or β -D-glucopyranose tetramethyl ether (synonym: 2,3,4,6-tetra-O-methyl-β-D-glucose) II. β-D-Glucopyranose 3-methyl ether (synonym: 3-Omethyl- β -p-glucopyranose)

Rule 14.—When a prefix is attached to one of the words in a two- or three-word name, it modifies only the word to which it is attached and does not modify the remaining words in the name. But if a preceding word in this name is the name of a compound, numerals to indicate positions of substitution in it may be placed before the following word (see Rule 11). If necessary, parentheses should be used to avoid ambiguity.

Unless otherwise specified (Rules 15 and 17), prefixes take an alphabetical order, regardless of the numerical prefix of each; a compound-radical name is treated as a unit. Thus, triacetyl and diacetyl are to be listed under acetyl. Anhydro and deoxy are subject to alphabeting under "a" and "d," respectively.

COMMENT.—This is in conformity with established usage: for example, CH₃OCH₂CO₂CH₃: methyl methoxyacetate. Examples:

Methyl 2,3,4,6-tetra-O-methyl- α -D-glucoside

Methyl 6-O-benzoyl- α -D-glucopyranoside

Ethyl 2,3,4-tri-O-acetyl-6-O-(phenylsulfonyl)-α-D-glucoside Methyl 3-O-(2-chloroethyl)-\beta-D-glucopyranoside

Rule 15.—The anomeric prefix (α - or β -), which can only be used in conjunction with a configurational prefix (D or L), will immediately precede the latter. The configurational prefix will directly precede the stem name (see Rule 6).

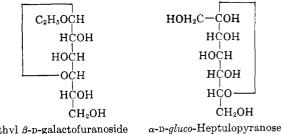
COMMENT.-In the D-series, the more dextrorotatory anomer of a glycose is designated α and the hemiacetal hydroxyl group (or derivative thereof) on the anomeric carbon atom is written to the right in the Fischer projection formula; the less dextrorotatory anomer is designated β and its corresponding anomeric group is written to the left in the Fischer projection formula. The reverse holds for the α and β anomers in the \bot series.

The steric arrangement of the groups on the α -D anomeric carbon atom is the same as that on the β -L anomeric carbon atom; that on the α -L anomeric carbon atom is the same as that on the β -D anomeric carbon atom. In a few accepted trivial names (see the third example below), the configurational prefix is understood and may be omitted.

The significant point is the absolute configuration of the anomeric carbon atom in relation to that of the configurational carbon atom (see Rules 5 and 22), the α forms being, in this respect, configurationally *cis* and the β forms *trans*.

Examples:

Methyl α -D-glucopyranoside ($[\alpha]^{20}D + 158^{\circ}$ in water) Methyl α -L-glucopyranoside ($[\alpha]^{20}_{D} - 158^{\circ}$ in water) Methyl β -cellobiopyranoside



Ethyl β -D-galactofuranoside

Rule 16.—In conformity with established practice, hyphens will be used in names to connect letters or numerals to syllables, or to separate different kinds of characters, such as Roman letters from Greek letters or letters from numerals.

The preferred style is to connect syllables directly (no hyphens). Hyphens may be inserted, however, for the sake of clarity.

Examples: α-D-Glucose 3-O-Methyl-β-L-mannose Penta-O-acetyl-α-D-glucopyranose Methyl 2,3,6-tri-O-acetyl-α-D-glucopyranoside 1,3:4,6-Di-O-methylenegalactitol (see Rule 31) 2-O-Methyl-3,4-dimethyl-β-D-glucopyranose

Rule 17.—The acyclic nature of a sugar or derivative containing an uncyclized CHO or CO group as the primary function will be indicated by inserting the italicized prefix *aldehydo* or *keto*, respectively, immediately before the configurational prefix and stem name.

Examples:

aldehydo-D-Glucose pentaacetate 3,6-Anhydro-aldehydo-D-galactose keto-D-Fructose pentabenzoate Penta-O-acetyl-aldehydo-D-glucose oxime

Rule 18.—The size of the ring in the heterocyclic forms of monosaccharides (both aldoses and ketoses) may be indicated by replacing, in the sugar name, the letters "se" by "furanose" for the 5-atom ring, "pyranose" for the 6-atom ring, and "septanose" for the 7-atom ring. Likewise, for the glycosides (both aldosides and ketosides), the size of the ring may be revealed by replacing the syllable "-side" by "furanoside," "pyranoside," or "septanoside."

Examples:

1,2-O-Isopropylidene- β -L-idofuranose Methyl β -D-altro-heptulopyranoside

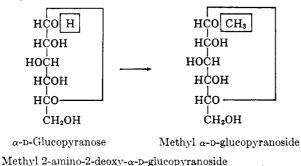
Rule 19.—The root "glyc" (as in glycose or glycoside) will be used in a generic sense to denote any sugar or derivative thereof, rather than some specified sugar.

Examples:

 $\begin{array}{c|c} Glycose & | generic \\ Methyl glycoside \\ \beta-L-Glucose \\ Methyl \alpha-D-glucofuranoside \\ Ethyl \beta-D-altropyranoside \\ Methyl \beta-L-fructofuranoside \\ \beta-D-Fructose \\ \end{array} \right\}$

Rule 20.—A glycoside is a mixed acetal resulting from the exchange of an alkyl or aryl radical for the hydrogen atom of the hemiacetal hydroxyl group of a cyclic form of an aldose or ketose. It is named by substituting "ide" as a suffix in place of the terminal "e" of the corresponding sugar name and placing before this word, separated by a space, the name of the organic substituent.

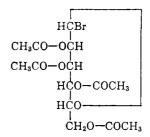
Examples:



Rule 21.—If the hemiacetal hydroxyl group is detached from a cyclic modification of an aldose or ketose, the residue is a glycosyl (glycofuranosyl, glycopyranosyl, glycoseptanosyl) radical. It is named by substituting "yl" as a suffix in place of the terminal "e" of the corresponding sugar name.

COMMENT.—A glycosyloxy radical is identical with a glycoside radical (see Rule 20).

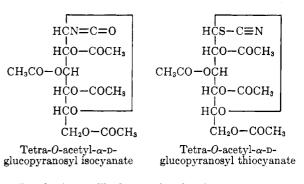
Examples:



Tetra-O-acetyl-α-D-mannopyranosyl bromide

 α -D-Glucopyranosyl dihydrogen phosphate [or α -D-glucopyranose 1-(dihydrogen phosphate)]

 β -D-Glucopyranosyluronic acid benzoate (or 1-O-benzoyl- β -D-glucopyranuronic acid) (see Rule 27)



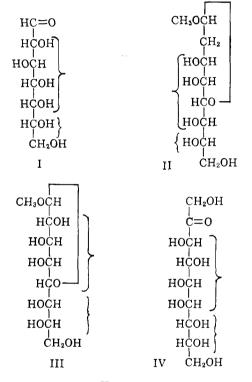
D-Ribosylamine 5-(dihydrogen phosphate) N-Methyl-6-O-methyl- β -L-talofuranosylamine N-Phenyl- α -D-glucopyranosylamine N- α -D-Glucopyranosylhydroxylamine

Rule 22.—A monosaccharide containing more than four configurational asymmetric carbon atoms will be named by adding two or more prefixes, indicating the configurations of those asymmetric carbon atoms, to a root indicating the number of carbon atoms in the chain and ending with the suffix "-ose" for aldoses and "-ulose" for ketoses.

The configurational prefixes employed are given in Rule 6. For the aldoses and 2-ketoses, the sequence of asymmetric carbon atoms will be divided into units, commencing, with a unit of four asymmetric carbon atoms, at the asymmetric carbon atom next to the functional group (see below). The order of citation of these prefixes will commence at the end farthest from carbon atom number one, and proceed along the carbon chain to the asymmetric carbon atom nearest to carbon atom number one. In designating the anomeric ring forms of these aldoses and 2-ketoses, the anomeric prefix here (see Rule 15) will immediately precede the configurational prefix for that group of asymmetric carbon atoms, next to the functional group, which has one or more atoms involved in the ring.

Number of asymmetric carbons in the sequence	Order of selection	to be used Order of citation
5	one 4-carbon +	one 1-carbon +
-	one 1-carbon	one 4-carbon
6	one 4-carbon +	one 2-carbon $+$
	one 2-carbon	one 4-carbon
7	one 4-carbon $+$	one 3-carbon +-
	one 3-carbon	one 4-carbon
8	two 4-carbon	two 4-carbon
9	two 4-carbon +	one 1-carbon $+$
	one 1-carbon	two 4-carbon
10	two 4-carbon $+$	one 2-carbon $+$
	one 2-carbon	two 4-carbon
11, etc.	two 4-carbon +	one 3-carbon $+$
	one 3-carbon, etc.	two 4-carbon, etc.

Examples:

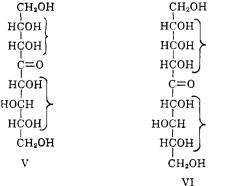


- D-glycero-D-gluco-Heptose Methyl 2-deoxy-1-glycero- α -L-gulo-octopyranoside Methyl 1-erythro- β -D-galacto-octopyranoside II.
- III.

IV. D-erythro-L-gluco-Nonulose

For other ketoses, the sequence of asymmetric carbon atoms will be similarly divided into units that commence with the group of three (or, if present, four) highest-numbered asymmetric carbon atoms that are next to the functional group. Examples:



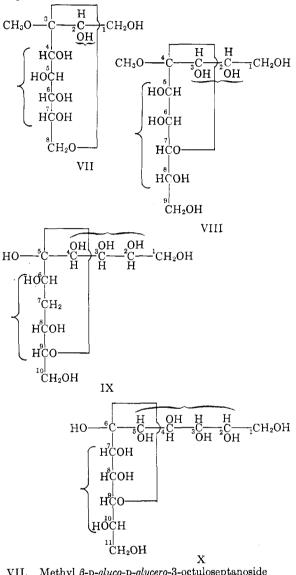


V. D-xylo-D-erythro-4-Octulose

VI. D-xylo-D-ribo-5-Nonulose or L-ribo-L-xylo-5-Nonulose

For oxygen-ring forms of ketoses other than 2-ketoses, the ending (furanose, furanoside, etc.) will, when necessary, be immediately preceded by a pair of numerals identifying the two carbon atoms to which the oxygen ring is attached, the potential ketone group being cited first. When the potential ketone group of an oxygen-ring form is in the middle of the chain, the anomeric carbon atom has, as usual, the top vertical orientation, and numbering proceeds downward and toward the ring-forming hydroxyl group.

Examples:



Methyl β -D-gluco-D-glycero-3-octuloseptanoside Methyl B-D-manno-D-erythro-4-nonulo-4,7-furanoside VIII. 7-Deoxy- β -D-arabino-L-ribo-5-deculo-5,9-pyranose

IX. X. a-L-talo-D-gulo-6-Undeculo-6,9-furanose

COMMENT.-If the carbonyl group is, with reference to the asymmetric carbon atoms, in the middle of the chain, the sugars resemble the alditols (Rule 23) and dialdoses (Rule 24), in that some are meso forms, for which the names are written without D or L, and some have two equally correct names (see example VI).

Rule 23 .-- Names for the polyhydric alcohols (alditols) are derived from the names of the corresponding aldose sugars by changing the suffix "ose" to "itol." For nonmeso compounds, the same family-determining asymmetric carbon atom as that characterizing the name of the sugar is used.

Examples:

⁽a) Names requiring D or L: threitol, arabinitol, glucitol, iditol, mannitol, rhamnitol, and talitol

(b) Names used without D or L: erythritol, ribitol, xylitol, allitol, and galactitol

The names of meso forms can be used advantageously with Dor L- in naming derivatives which have become optically active by substitution: 2,3-O-isopropylidene-D-xylitol, and 1,2-O-benzylidene-L-glycero-D-ido-heptitol.

(c) Cellobiitol, lactitol, and melibiitol

(d) Equivalent names:

D-Arabinitol and **D**-lyxitol

D-Glucitol and L-gulitol

n-Talitol and n-altritol

	toor and D-aton	1101			
(e) 	H₂OH	(CH₂OH	C	CH₂OH
нос	H	H	он	НÇ	юн
нç	HOH	нос	H	н	он
	2H₂OH)-Threitol; -threitol		CH₂OH -Threitol; -threitol		CH₂OH ∕thritol
(f)				CH ₂ O	H

		,	
(CH2OH	HOG	н
HOO	H	HO	ЮН
HC	он	HO	сон
HOO	н	HOO	H
HO	он	HO	он
HO	сон	HO	он
	CH ₂ OH	(CH2OH
D-glycero-D-	- <i>ido</i> -Heptitol	d-erythro-l-	galacto-Octitol
	or		or
D-glycero-L-	gulo-Heptitol	D-threo-L-	<i>gulo-</i> Octitol

(g) Some of the higher carbon polyhydric alcohols are meso forms and the names are written without D or L, but the prefix meso may be added to avoid ambiguity.

	CH_2OH
CH_2OH	нсон
нсон	нсон
носн	носн
нсон	носн
носн	нсон
нсон	нсон
CH2OH meso-glycero-ido-Heptitol	CH2OH meso-erythro-manno-Octitol

Rule 24.—Dialdehydes formed from aldoses having a terminal ---CH₂OH group by oxidation of this group only to -CHO may be named by attaching the suffix "dialdose" to a root indicating the number of carbon atoms in the chain and then adding prefixes indicating the configurations of the asymmetric carbon atoms.

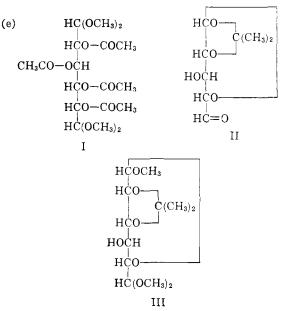
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(a)				HO	C==0
		н	2=0	HO	юн
HO	2=0	HOG	н	нос	H
HO	юн	HOO	H	но	он
нос	н	HOO	H	HO	он
)=0		=0		D==0
L-threo-Te	trodialdose	ribo-Pent	odialdose	D-gluco-He	xodialdose

- (b) Names requiring D or L: threo-tetrodialdose, arabinopentodialdose, gluco-hexodialdose, ido-hexodialdose, mannohexodialdose, and talo-hexodialdose.
- (c) Names of meso forms are used without D or L (the prefix meso- may be inserted for clarity): erythro-tetrodialdose, ribo-pentodialdose, xylo-pentodialdose, allo-hexodialdose, and meso-galactc-hexodialdose.

The names of meso forms can be used advantageously with D or L in naming derivatives which have become optically active by substitution.

(d) Equivalent names: D-arabino-Pentodialdose and D-lyxo-pentodialdose D-gluco-Hexodialdose and L-gulo-hexodialdose D-talo-Hexodialdose and D-altro-hexodialdose



T.

Tetra-O-acetyl-D-gluco-hexodialdose bis(dimethyl acetal) 1,2-O-Isopropylidene- α -D-xylo-pentodialdo-1,4-furanose Methyl 2,3-O-isopropylidene- α -D-gulo-hexodialdo-1,5-pyr-III. anoside 6-(dimethyl acetal)

Rule 25.—Aldonic acids, formed from aldoses by oxidation of only the hemiacetal or aldehydic carbon atom to --- CO-OH, may be named by substituting "onic acid" as a suffix in place of "ose" of the corresponding aldose name. Acid chlorides, amides, esters, lactones (see comment, Rule 28), nitriles, salts, and the like, are named in the conventional manner.

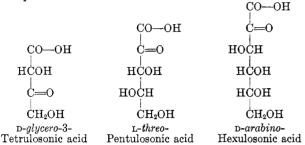
Examples:

- (a) Permissible names established by usage: cellobionic acid, lactobionic acid, and melibionic acid
- (b) Methyl tetra-O-acetyl-L-arabinonate or methyl L-arabinonate tetraacetate
 - Barium *D*-gluconate
 - Penta-O-acetyl-D-gluconic acid or D-gluconic acid pentaacetate
 - Penta-O-acetyl-D-galactonic acid monohydrate or D-galactonic acid pentaacetate monohydrate
 - D-Glucono-1,4-lactone or D-glucono- γ -lactone
 - D-Gluconic 1,4-lactone or D-gluconic γ -lactone
 - D-Glucono-1,5-lactone or D-glucono-δ-lactone
 - D-Gluconic 1,5-lactone or D-gluconic δ -lactone
 - 2,3,4,6-Tetra-O-methyl-L-altronolactone or 2,3,4,6-tetra-Omethyl-L-altronic lactone
- 2-Amino-2-deoxy-D-gluconic acid

Examples illustrating combination of Rules 11 and 25: Sodium D-gluconate 6-(dihydrogen phosphate) Sodium p-gluconate 6-(sodium hydrogen phosphate) Sodium D-gluconate 6-(disodium phosphate)

Rule 26.—When a secondary alcoholic hydroxyl group of an aldonic acid is oxidized to a carbonyl group, the compound will be named by means of the suffix "ulosonic acid" attached to a root designating the number of carbon atoms in the chain, which is in turn preceded by the appropriate numeral indicating the position of the ketonic function when other than 2 (see Rule 7). The configuration of the acid will be designated as given in Rule 6.

Examples:



α-D-arabino-Hexulopyranosonic acid (common name: 2-keto-D-gluconic acid)

 β -D-arabino-Hexulopyranosono-1,4-lactone

Methyl a-D-arabino-hexulopyranosidonic acid

Methyl β -D-arabino-hexulofuranosidonamide

Ethyl (methyl α -D-arabino-hexulopyranosid)onate

Sodium (ethyl a-D-arabino-hexulofuranosid)onate

Rule 27.—Uronic acids, formed from aldoses having a terminal —CH₂OH group by oxidation only of this group to —CO-OH, will be named by substituting "uronic acid" as a suffix in place of "ose" of the corresponding aldose name. The hemiacetal or aldehydic carbon atom is carbon number one, and the syllable "ur" has the significance of " ω ."

Acid chlorides, amides, esters, lactones (see Comment, Rule 28), nitriles, salts, and the like, are named in the conventional manner.

Examples:

- α -D-Mannopyranuronic acid
- Tetra-O-acetyl- β -D-talopyranuronic acid (or β -D-talopyranuronic acid tetraacetate)
- Methyl β -L-galactopyranuronate
- Sodium *a*-L-glucofuranuronate
- Ethyl tetra- \tilde{O} -benzoyl- α -D-idofuranuronate
- 3-O-Methyl-α-D-ribofuranurono-5,2-lactone
- α-D-Mannopyranurono-6,2-lactone
- 2-O-Ethvl- β -L-glucopyranurono- γ -lactone
- 2,3,4-Tri-O-acetyl-1-bromo-1-deoxy- α -D-glucuronic acid
- α -D-Glucopyranuronic acid 1-(dihydrogen phosphate) or α -Dglucopyranosyluronic acid dihydrogen phosphate

Rule 28.—If the glycoside radical (see Rule 20) of an aldose glycoside possesses a terminal —CH₂OH group, and, if this group of the glycoside is oxidized to a carboxyl group, the product will be named by substituting "uronic acid" as a suffix in place of the terminal "e" of the parent glycoside name. The glycosidic hemiacetal carbon atom is carbon number one, and the syllable "ur" has the significance of " ω ."

Acid chlorides, amides, esters, lactones (see Comment), nitriles, salts, and the like, are named in the conventional manner.

COMMENT.—Parentheses are suitably inserted where it is necessary to distinguish between an ester alkyl group and the hemiacetal alkyl group of a glycoside of a uronic acid. In numbering lactones, the first number refers to the position of the carbonyl carbon atom.

Examples:

- Methyl α -D-mannopyranosiduronic acid
- Ethyl tri-O-benzoyl-α-D-idofuranosiduronic acid
- Methyl α -D-glucopyranosidurono-6,3-lactone (or γ -lactone)
- Ethyl 3-O-ethyl- β -L-glucopyranosidurono-6,2-lactone (or δ -lactone)

Ethyl (methyl β -L-galactopyranosid)uronate Sodium (bornyl α -D-glucofuranosid)uronate Butyl (propyl tri-O-acetyl- β -D-talopyranosid)uronate Methyl (ethyl 2,3,4-tri-O-methyl- α -D-galactosid)uronate

Rule 29.—Dicarboxylic sugar acids (aldaric acids), formed by the oxidation of aldoses at both terminal carbon atoms, will be named by substituting "aric acid" as a suffix in place of "ose" of the corresponding aldose name.

Examples:

- (a) Permissible names established by usage:
 - dextro-Tartaric acid for L-threaric acid
- meso-Tartaric acid for erythraric acid
- (b) Names requiring D or L: threaric acid, arabinaric acid, glucaric acid, idaric acid, mannaric acid, and talaric acid
- (c) Names used without D or L: erythraric acid, ribaric acid, xylaric acid, allaric acid, and galactaric acid

The names of meso forms can be used advantageously with D or L in naming derivatives which have become optically active by substitution (see Rule 23b).

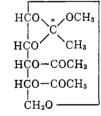
(d) Equivalent names:

Lyxaric acid and arabinaric acid L-Gularic acid and D-glucaric acid

Talaric acid and altraric acid

Rule 30.—The "glycosides of ortho ester structure" may be named as the ortho esters, with the carbohydrate group given as the first term in the name.

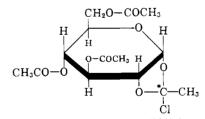
Examples: (a)



D-Ribose 1,2-(methyl orthoacetate) 3,4-diacetate

It is to be noted that this compound may also be named according to Rule 31 as 3,4-di-O-acetyl-1,2-O-(1-methoxyethylidene)-Dribose. This latter system appears to be the best one for assigning an accurate name to the following compound:

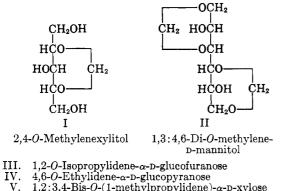




 $3,4,6\text{-}\mathrm{Tri}\text{-}O\text{-}\mathrm{acetyl}\text{-}1,2\text{-}O\text{-}(1\text{-}\mathrm{chloroethylidene})\text{-}\alpha\text{-}\mathrm{D\text{-}glucose}$

COMMENT.—These two examples contain the asymmetric carbon atom marked with *, and so two forms are possible. No recommendations are made at present for their differentiation.

Rule 31.—Cyclic acetals formed by the reaction of carbohydrates with aldehydes or ketones may be named in accordance with Rule 9 with bivalent radicals as prefixes, such radicals to follow the nomenclature set forth in International Union of Pure and Applied Chemistry (I.U.P.A.C.) Rule 56.1. In representing more than one cyclic acetal grouping, the numeral pairs are separated typographically when the exact placement of the acetal groups is known. Examples:



1,2:3,4-Bis-O-(1-methylpropylidene)- α -D-xylose

VI. Methyl 4,6-O-benzylidene- α -D-glucopyranoside

VII. $1,2-O-(2-Chloroethylidene)-\alpha-D-glucofuranose$ VIII. 1,2-O-(1-Chloroethylidene)-a-D-glucopyranose triacetate

COMMENT.--It is to be noted that in Examples IV to VIII, inclusive, new asymmetric centers are introduced at the carbonyl carbon atom of the aldehyde or ketone that has reacted with the sugar. In V, two such new centers have been introduced. A differentiating nomenclature for such isomers is not here attempted.

Rule 32.—In naming acetals formed between alcohols (or thiols) and the carbonyl carbon atom of the acyclic forms of aldoses or ketoses, the name of the sugar will be the first word, "acetal" ("dithioacetal") the last word, and the name of the appropriate radical (or radicals) will be the middle word (or words). Derivatives containing the hemiacetal function are named in an analogous manner.

Examples:

anipies,				
$\mathrm{HC}(\mathrm{OC}_{2}\mathrm{H}_{5})_{2}$	CH_2OH	$\operatorname{HC}_{ }(\operatorname{SC}_{2}\operatorname{H}_{5})_{2}$	$_{\rm H_2OH}$	
HCOH	$\overset{1}{\mathrm{C}}(\mathrm{OC}_{2}\mathrm{H}_{5})_{2}$	нсон	$\overset{ }{\mathrm{C}}(\mathrm{SC}_{2}\mathrm{H}_{5})_{2}$	
носн	носн	носн	носн	
нсон	нсон	нсон	нсон	
нсон	нсон	нсон	нсон	
$\rm CH_2OH$	$\dot{\mathrm{CH}}_{2}\mathrm{OH}$	$\dot{\mathrm{CH}}_{2}\mathrm{OH}$	$\rm CH_2OH$	
D-Glucose	D-Fructose	D-Glucose	p-Fructose	
${f diethyl} \\ {f acetal}$	$\begin{array}{c} {f diethyl} \\ {f acetal} \end{array}$	diethyl	diethyl	
		dithioacetal	dithioacetal	
sc	L_2H_b	Se	C_2H_5	
нċс	$C_{2}H_{5}$	нĊ	OCH3	
нсо	θH	HC	ЭH	
носн		HOCH		
HCOH		нÇ	OH	
HCOH		нÇ	OH	
CH	I2OH	Ċ	H ₂ OH	
p-Glucose diethyl		D- Glucose	S-ethyl O-	
monothioacetal		methyl mor	nothioacetal	
OC_2H_5		S	C_2H_5	
нĊ	HC	HCOH		
нĊ	$O-COC_6H_5$	$\mathbf{H}_{\mathbf{L}}^{\mathbf{L}}$	OCOCH3	
C ₆ H ₅ COOCI	H	CH ₃ CO-OC	н	
нÇ	$O-COC_6H_5$	CH ₃ CO-OC	Н	
HCO-COC ₆ H ₅		HC	O-COCH3	
ĊI	H ₂ O—COC ₆ H ₅	\mathbf{C}	H ₂ OCOCH ₃	
2,3,4,5,6-Penta-O-benzoyl- D-glucose ethyl hemiacetal		2,3,4,5,6-Penta- O -acetyI-D- galactose S-ethyl monothio- hemiacetal		

COMMENT.-In the last four examples above, carbon atom number one has become asymmetric and two forms are possible. No recommendations are made at present for their differentiation.

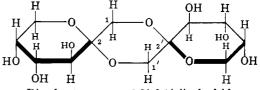
Rule 33.—An intramolecular anhydride, formed by the elimination of the elements of water from two hydroxyl groups of a monosaccharide molecule (aldose or ketose), is named by attaching by a hyphen before the sugar name the prefix "anhydro"; this, in turn, is preceded by a pair of numerals identifying the two hydroxyl groups involved. Anhydrides of sugar acids, alcohols, lactones, and the like, are named similarly.

COMMENT.-The substances usually known as sugar anhydrides, glycose anhydrides, or glycosans (whose formation involves the reducing group), as well as the anhydro sugars (whose formation does not involve the reducing group) are not here differentiated in treatment. The names "levoglucosan" (for 1,6anhydro- β -D-glucopyranose) and "sedoheptulosan" (for 2,7anhydro- β -D-altro-heptulopyranose) are established by usage, but, except for this, names of glucosan type should not be used. Examples:

- 3,6-Anhydro-aldehydo-D-glucose
- 3,6-Anhydro-β-D-glucofuranose
- 2,3-Anhydro-4-O-methyl- α -D-mannopyranose
- 1,7-Anhydro-D-glycero-β-D-gulo-heptopyranose
- 1,6:3,4-Dianhydro- β -D-talose
- Methyl 4,6-di-O-acetyl-2,3-anhydro- α -D-alloside
- 2,5-Anhydro-D-gluconic acid
- 3,6-Anhydro-D-gluconic 1,4-lactone or 3,6-anhydro-D-glucono-1,4-lactone
- 1,4:3,6-Dianhydro-D-glucitol or 1,4:3,6-dianhydro-L-gulitol (see Rule 23)

Rule 34.—An intermolecular anhydride, formed by condensation of two monosaccharide molecules with the elimination of the elements of two molecules of water, will be named by the word "dianhydride" placed after the names of the two parent sugars. The position of each anhydride link is indicated by a pair of numerals showing the positions of the two hydroxyl groups involved; the numerals relating to one sugar (in a mixed dianhydride, the second sugar named) will be primed. Both pairs of numerals will immediately precede the word "dianhydride."

Examples:



Di-D-fructopyranose 1,2':2,1'-dianhydride

Di-β-D-fructofuranose 1,2':2,3'-dianhydride

 β -D-Fructofuranose β -D-threo-pentulofuranose 1,2':2,1'-dianhydride

Di-D-ribofuranose 1,5':1',5-dianhydride

Rule 35.—An oligosaccharide is a compound which. on complete hydrolysis, gives monosaccharide units only, in relatively small number per molecule (in contrast to the high-polymeric polysaccharides).

COMMENT.---Most of the naturally occurring oligosaccharides have well-established and useful common names (cellobiose, lactose, maltose, melezitose, raffinose, stachyose, and sucrose) which were assigned before their complete structures were known. Rational names may now be assigned as follows.

Disaccharides.—A nonreducing disaccharide may be named as a glycosyl glycoside, and a reducing disaccharide as a glycosylglycose, from its component parts. A reducing disaccharide may also be named according to the system described below for the tri- and higher oligo-saccharides.

Examples:

(a) Nonreducing

Sucrose: β -D-fructofuranosyl α -D-glucopyranoside or α -D-glucopyranosyl β -D-fructofuranoside

(b) Reducing α -Lactose: 4-O- β -D-galactopyranosyl- α -D-glucopyranose or O- β -D-galactopyranosyl- $(1 \rightarrow 4)$ - α -D-glucopyranose

- (c) Derivatives of reducing disaccharides
- I. Methyl α -lactoside: methyl 4-O- β -D-galactopyranosyl- α -D-glucopyranoside or methyl O- β -D-galactopyranosyl- $(1 \rightarrow 4)$ - α -D-glucopyranoside
- II. 2-Amino-2-deoxy-4- $O(\beta$ -D-galactopyranosyl)- α -D-gluco-pyranose or $O-\beta$ -D-galactopyranosyl- $(1 \rightarrow 4)$ -2-amino-2-deoxy- α -D-glucopyranose
- III. 3-O-(4-O-Methyl- α -D-galactopyranosyluronic acid)- α -D-glucopyranose or O-(4-O-methyl- α -D-galactopyranosyluronic acid)-(1 \rightarrow 3)- α -D-glucopyranose
- IV. 3-O-(2-Amino-2-deoxy- β -D-glucopyranosyl)- α -D-glucopyranuronic acid or O-(2-amino-2-deoxy- β -D-glucopyranosyl)-(1 \rightarrow 3)- α -D-glucopyranuronic acid
- V. 6-O-(Methyl tri-O-acetyl- β -D-mannopyranosyluronate)-tri-O-acetyl- α -D-altropyranosyl bromide or O-(methyl tri-Oacetyl- β -D-mannopyranosyluronate)-(1 \rightarrow 6)-tri-O-acetyl- α -D-altropyranosyl bromide
- VI. 4-O-(Methyl 4-O-methyl- α -D-glucopyranosyluronate)- α -D-xylopyranose or O-(methyl 4-O-methyl- α -D-glucopyranosyluronate)-(1 \rightarrow 4)- α -D-xylopyranose
- VII. Phenyl 2-amino-2-deoxy-3-O-(ethyl β -D-glucopyranosyluronate)- β -D-galactopyranoside or phenyl O-(ethyl β -Dglucopyranosyluronate)-(1 \rightarrow 3)-2-amino-2-deoxy- β -D-galactopyranoside

Tri- and Higher Oligo-saccharides

(a) Nonreducing

Raffinose: $O_{-\alpha-D}$ -galactopyranosyl- $(1 \rightarrow 6)_{-\alpha-D}$ -glucopyranosyl β -D-fructofuranoside

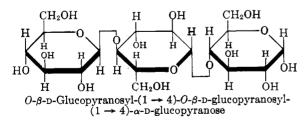
Gentianose: O- β -D-glucopyranosyl- $(1 \rightarrow 6)$ - α -D-glucopyranosyl β -D-fructofuranoside

(b) Reducing

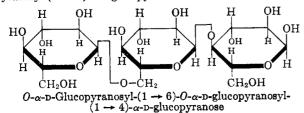
Beginning with the first nonreducing component, and following Rule 21, the first glycosyl portion with its configurational prefixes is delineated. This is followed by two numbers which indicate the respective positions involved in this glycosidic union; these numbers are separated by an arrow (pointing from the glycosyl carbon atom number to the number for the hydroxylic carbon atom involved) and are enclosed in parentheses inserted into the name by hyphens. The next disaccharide linkage is treated similarly (and so on), and the last portion of the name delineates the reducing sugar unit.

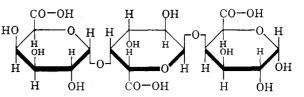


 α -Cellotriose:



 α -Maltotriose: $O \cdot \alpha$ -D-glucopyranosyl- $(1 \rightarrow 4)$ - $O \cdot \alpha$ -D-glucopyranosyl- $(1 \rightarrow 4)$ - α -D-glucopyranose

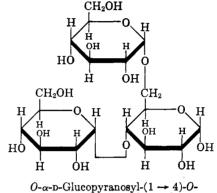




 $O\text{-}(\alpha\text{-}\text{D}\text{-}\text{Galactopyranosyluronic}$ acid)-(1 \rightarrow 4)- $O\text{-}(\alpha\text{-}\text{D}\text{-}\text{galactopyranosyluronic}$ acid)-(1 \rightarrow 4)- $\alpha\text{-}\text{D}\text{-}\text{galactopyranuronic}$ acid

Reducing, branched

By inserting one glycosyl substituent in brackets, it is distinguished from the second glycosyl substituent.



 $\begin{array}{l} O\text{-}\alpha\text{-}\text{D-}\text{Glucopyranosyl-}(1\rightarrow 4)\text{-}O\text{-}\\ [\alpha\text{-}\text{D-}\text{glucopyranosyl-}(1\rightarrow 6)]\text{-}\alpha\text{-}\text{D-}\text{glucopyranose} \end{array}$

Synonym: 4, 6-di-O-(α -D-glucopyranosyl)- α -D-glucopyranose

APPENDIX

Conventions Regarding Symbols for Representing Complex Carbohydrates

In abbreviated, structural representation of complex carbohydrates, the following symbols may be convenient.

(1) Radicals derived from monosaccharides.—For trioses to hexoses, the first three letters of the name are used; an exception is that "glucose" is denoted by G. The first of the three letters is capitalized.

Examples:

Galactose, Gal; fructose, Fru; ribose, Rib; 2-deoxy-D-erythropentose, 2-deoxyRib

(2) Furanose, pyranose, and septanose forms.—If necessary, the first letter of the syllable, italicized and uncapitalized, is used as suffix to denote the ring form.

Examples:

Idofuranose, Idof; mannopyranose, Manp

(3) Uronic acids.—The suffix "A" (for "acid") is added to the symbol for the parent monosaccharide.

Examples:

Galactofuranuronic acid, GalfA; mannopyranuronic acid, ManpA

(4) 2-Amino-2-deoxyaldoses.—The suffix "N" (for "nitrogen") is added to the symbol for the parent monosaccharide. The N-acetyl derivative is denoted by the suffix NAc.

Examples:

2-Amino-2-deoxy-D-glucose, GN; 2-acetamido-2-deoxy-D-galactose, GalNAc

(5) Configurational series.—The configurational symbols (Rule 4) are not to be omitted when established.

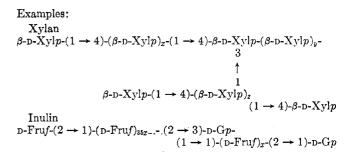
Example:

L-arabinose, L-Ara

(6) **Positional numerals and anomeric prefixes.**—These are added at the appropriate places, the former being separated by arrows pointing from the glycosyl group to the hydroxyl group which is substituted thereby.

(7) Joining of symbols.—Symbols formed as above are joined by hyphens.

(8) Arrays.—Polydirectional arrays may be used.



ADDENDUM TO "DEFINITIVE RULES FOR THE NOMENCLATURE OF NATURAL AMINO ACIDS AND RELATED SUBSTANCES"¹

This rule was proposed by Dr. H. B. Vickery who was largely responsible for the original report. The rule has been approved by the Committee on Nomenclature, Spelling, and Pronunciation of The American Chemical Society and by the Council of The American Chemical Society in March, 1962, on a tentative basis for at least one year. It was previously approved by the National Research Council Subcommittee on Biochemical Nomenclature and informally approved by the National Research Council Committee on Nomenclature and by the Division Committee on Carbohydrate Nomenclature of The American Chemical Society.

AA-11. A Rule for Naming α -Amino Acids which Have Two or More Centers of Asymmetry

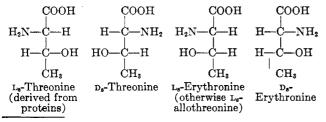
Names of α -amino acids which have two or more centers of asymmetry and in which a hydrogen atom is attached to each asymmetric carbon atom may be formed with use of the prefixes of carbohydrate nomenclature to define the configurational relationships. The small capital letter prefixes L. or D. are placed immediately before the name of the parent α -amino acid or its radical. The subscripts must invariably be inserted in order to show that the capital letter prefix refers to the configuration of the α -carbon atom (carbon atom 2). The carbohydrate name prefix is italicized in print.

Examples: The four optically active 3-hydroxyaspartic acids may be formulated according to the Fischer conventions and named as follows:

COOH	COOH	COOH	COOH
H₂NCH	H-C-NH2	H₂NCH	HCNH₂
носн	н—с—он	H-C-OH	HO-C-H
соон	соон	соон	COOH
erythro-3-	erythro-3-	threo-3-	threo-3-
Hydroxy-L_	Hydroxy-Ds-	Hydroxy-L _s -	Hydroxy-D ₈ -
aspartic acid	aspartic acid	aspartic acid	aspartic acid
(related to meso-tartaric	(related to <i>meso</i> -tartaric	[related to (-)-tartaric	[related to
acid)	acid)	acid]	(+)-tartaric acid]
actu)	acra/	actal	actual l

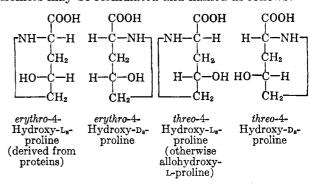
 L_s -Threenine was so named in order to define the configurational relationships of both asymmetric centers. Its diastereomer hitherto called L_s -allothreenine may accordingly be named L_s -erythronine.

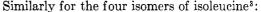
The formulas of the two pairs of enantiomorphs are as follows:

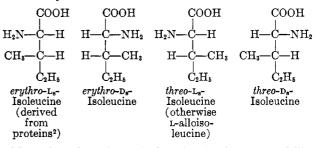




Since the configurational relationships of both asymmetric centers of hydroxyproline are known,² the isomers may be formulated and named as follows:







Note that these formulations imply the acceptability of a precedence convention according to which a smaller alkyl group is preferred to a larger. Alternatively, the formulas may be regarded as being written with the longest possible hydrocarbon chain.

The configurational relationships of the hydroxylysines have not at present been confirmed,⁴ but the isomers may be formulated and named as follows:

(2) The formulation is based upon the assignment of configuration by A. Neuberger [J. Chem. Soc., 429 (1945)] and by L. Benoiton, M. Winitz, S. M. Birnbaum, and J. P. Greenstein [J. Am. Chem. Soc., 79, 6192 (1957)], and recently confirmed by the studies of E. Adams and A. Goldstone [J. Biol. Chem., 235, 3504 (1960)].

(3) The formulation is based upon the assignment of the absolute configuration by J. Trommel and J. M. Bijvoet [Acta Cryst., 7, 703 (1954)] who employed X-ray crystallographic methods, and also upon the studies of J. P. Greenstein, L. Levintow, C. G. Baker, and J. White [J. Biol. Chem., 185, 647 (1951)] and of W. S. Fones [J. Am. Chem. Soc., 76, 1377 (1954)].

(4) B. Witkop [Experientia, 12, 372 (1956)] assigns the structure erythro-5-hydroxy-L₂-lysine to the amino acid from proteins, but this assignment has not been confirmed by other investigators.