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NOMENCLATURE OF CARBOHYDRATES (Recommendations 1996)

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Preamble

These Recommendations expand and replace the Tentative Rules for Carbohydrate Nomenclature [1] issued in 1969 jointly by the IUPAC Commission on the Nomenclature of Organic Chemistry and the IUB-IUPAC Commission on Biochemical Nomenclature (CBN) and reprinted in [2]. They also replace other published JCBN Recommendations [3-7] that deal with specialized areas of carbohydrate terminology; however, these documents can be consulted for further examples. Of relevance to the field, though not incorporated into the present document, are the following recommendations:

Nomenclature of cyclitols, 1973 [8]

Numbering of atoms in *myo*-inositol, 1988 [9]

Symbols for specifying the conformation of polysaccharide chains, 1981 [10]

Nomenclature of glycoproteins, glycopeptides and peptidoglycans, 1985 [11]

Nomenclature of glycolipids, in preparation [12]

The present Recommendations deal with the acyclic and cyclic forms of monosaccharides and their simple derivatives, as well as with the nomenclature of oligosaccharides and polysaccharides. They are additional to the Definitive Rules for the Nomenclature of Organic Chemistry [13,14] and are intended to govern those aspects of the nomenclature of carbohydrates not covered by those rules.

2-Carb-0. Historical development of carbohydrate nomenclature [15]

2-Carb-0.1. Early approaches

In the early nineteenth century, individual sugars were often named after their source, e.g. grape sugar (Traubenzucker) for glucose, cane sugar (Rohrzucker) for saccharose (the name sucrose was coined much later). The name glucose was coined in 1838; Kekulé in 1866 proposed the name 'dextrose' because glucose is dextrorotatory, and the laevorotatory 'fruit sugar' (Fruchtzucker, fructose) was for some time named 'laevulose' (American spelling 'levulose'). Very early, consensus was reached that sugars should be named with the ending '-ose', and by combination with the French word 'cellule' for cell the term cellulose was coined, long before the structure was known. The term 'carbohydrate' (French 'hydrate de carbone') was applied originally to monosaccharides, in recognition of the fact that their empirical composition can be expressed as $C_n(H_2O)_n$. However the term is now used generically in a wider sense (see 2-Carb-1.1).

2-Carb-0.2. The contribution of Emil Fischer

Emil Fischer [16] began his fundamental studies on carbohydrates in 1880. Within ten years, he could assign the relative configurations of most known sugars and had also synthesized many sugars. This led to the necessity to name the various compounds. Fischer and others laid the foundations of a terminology still in use, based on the terms triose, tetrose, pentose, and hexose. He endorsed Armstrong's proposal to classify sugars into aldoses and ketoses, and proposed the name fructose for laevulose, because he found that the sign of optical rotation was not a suitable criterion for grouping sugars into families.

The concept of stereochemistry, developed since 1874 by van't Hoff and Le Bel, had a great impact on carbohydrate chemistry because it could easily explain isomerism. Emil Fischer introduced the classical projection formulae for sugars, with a standard orientation (carbon chain vertical, carbonyl group at the top); since he used models with flexible bonds between the atoms, he could easily 'stretch' his sugar models into a position suitable for projection. He assigned to the dextrorotatory glucose (via the derived glucaric acid) the projection with the OH group at C-5 pointing to the right, well knowing that there was a 50% chance that this was wrong. Much later (Bijvoet, 1951), it was proved correct in the absolute sense.

Rosanoff in 1906 selected the enantiomeric glyceraldehydes as the point of reference; any sugar derivable by chain lengthening from what is now known as D-glyceraldehyde belongs to the D series, a convention still in use.

2-Carb-0.3. Cyclic forms

Towards the end of the nineteenth century it was realized that the free sugars (not only the glycosides) existed as cyclic hemiacetals or hemiketals. Mutarotation, discovered in 1846 by Dubrunfaut, was now interpreted as being due to a change in the configuration of the glycosidic (anomeric) carbon atom. Emil Fischer assumed

the cyclic form to be a five-membered ring, which Tollens designated by the symbol <1,4>, while the six-membered ring received the symbol <1,5>.

In the 1920s, Haworth and his school proposed the terms 'furanose' and 'pyranose' for the two forms. Haworth also introduced the 'Haworth depiction' for writing structural formulae, a convention that was soon widely followed.

2-Carb-0.4. Nomenclature commissions

Up to the 1940s, nomenclature proposals were made by individuals; in some cases they were followed by the scientific community and in some cases not. Official bodies like the International Union of Chemistry, though developing and expanding the Geneva nomenclature for organic compounds, made little progress with carbohydrate nomenclature. The IUPAC Commission on Nomenclature of Biological Chemistry put forward a classification scheme for carbohydrates, but the new terms proposed have not survived. However in 1939 the American Chemical Society (ACS) formed a committee to look into this matter, since rapid progress in the field had led to various misnomers arising from the lack of guidelines. Within this committee, the foundations of modern systematic nomenclature for carbohydrates and derivatives were laid: numbering of the sugar chain, the use of D and L and α and β , and the designation of stereochemistry by italicized prefixes (multiple prefixes for longer chains). Some preliminary communications appeared, and the final report, prepared by M.L. Wolfrom, was approved by the ACS Council and published in 1948 [17].

Not all problems were solved, however, and different usages were encountered on the two sides of the Atlantic. A joint British-American committee was therefore set up, and in 1952 it published 'Rules for Carbohydrate Nomenclature' [18]. This work was continued, and a revised version was endorsed in 1963 by the American Chemical Society and by the Chemical Society in Britain and published [19]. The publication of this report led the IUPAC Commission on Nomenclature of Organic Chemistry to consider the preparation of a set of IUPAC Rules for Carbohydrate Nomenclature. This was done jointly with the IUPAC-IUB Commission on Biochemical Nomenclature, and resulted in the 'Tentative Rules for Carbohydrate Nomenclature, Part I, 1969', published in 1971/72 in several journals [1]. It is a revision of this 1971 document that is presented here. In the present document, recommendations are designated 2-Carb-*n*, to distinguish them from the Carb-*n* recommendations in the previous publication.

2-Carb-1. Definitions and conventions

2-Carb-1.1. Carbohydrates

The generic term 'carbohydrate' includes monosaccharides, oligosaccharides and polysaccharides as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxy group(s) by a hydrogen atom, an amino group, a thiol group or similar heteroatomic groups. It also includes derivatives of these compounds. The term 'sugar' is frequently applied to monosaccharides and lower oligosaccharides. It is noteworthy that about 3% of the compounds listed by Chemical Abstracts Service (i.e. more than 360 000) are named by the methods of carbohydrate nomenclature.

Note. Cyclitols are generally not regarded as carbohydrates. Their nomenclature is dealt with in other recommendations [8,9].

2-Carb-1.2. Monosaccharides

Parent monosaccharides are polyhydroxy aldehydes $\text{H}-(\text{CHOH})_n-\text{CHO}$ or polyhydroxy ketones $\text{H}-(\text{CHOH})_n-\text{CO}-(\text{CHOH})_m-\text{H}$ with three or more carbon atoms.

The generic term 'monosaccharide' (as opposed to oligosaccharide or polysaccharide) denotes a single unit, without glycosidic connection to other such units. It includes aldoses, dialdoses, aldoketoses, ketoses and diketoses, as well as deoxy sugars and amino sugars, and their derivatives, provided that the parent compound has a (potential) carbonyl group.

1.2.1. Aldoses and ketoses

Monosaccharides with an aldehydic carbonyl or potential aldehydic carbonyl group are called aldoses; those with a ketonic carbonyl or potential ketonic carbonyl group, ketoses.

Note. The term 'potential aldehydic carbonyl group' refers to the hemiacetal group arising from ring closure. Likewise, the term 'potential ketonic carbonyl group' refers to the hemiketal structure (see 2-Carb-5).

1.2.2. Cyclic forms

Cyclic hemiacetals or hemiketals of sugars with a five-membered (tetrahydrofuran) ring are called furanoses, those with a six-membered (tetrahydropyran) ring pyranoses. For sugars with other ring sizes see 2-Carb-5.

2-Carb-1.3. Dialdoses

Monosaccharides containing two (potential) aldehydic carbonyl groups are called dialdoses (see 2-Carb-9).

2-Carb-1.4. Diketoses

Monosaccharides containing two (potential) ketonic carbonyl groups are termed diketoses (see 2-Carb-11).

2-Carb-1.5. Ketoaldoses (aldoketoses, aldulososes)

Monosaccharides containing a (potential) aldehydic group and a (potential) ketonic group are called ketoaldoses (see 2-Carb-12); this term is preferred to the alternatives on the basis of 2-Carb-2.1.1 (aldose preferred to ketose).

2-Carb-1.6. Deoxy sugars

Monosaccharides in which an alcoholic hydroxy group has been replaced by a hydrogen atom are called deoxy sugars (see 2-Carb-13).

2-Carb-1.7 Amino sugars

Monosaccharides in which an alcoholic hydroxy group has been replaced by an amino group are called amino sugars (see 2-Carb-14). When the hemiacetal hydroxy group is replaced, the compounds are called glycosylamines.

2-Carb-1.8. Alditols

The polyhydric alcohols arising formally from the replacement of a carbonyl group in a monosaccharide with a CHO group are termed alditols (see 2-Carb-19).

2-Carb-1.9. Aldonic acids

Monocarboxylic acids formally derived from aldoses by replacement of the aldehydic group by a carboxy group are termed aldonic acids (see 2-Carb-20).

2-Carb-1.10. Ketoaldonic acids

Oxo carboxylic acids formally derived from aldonic acids by replacement of a secondary CHO group by a carbonyl group are called ketoaldonic acids (see 2-Carb-21).

2-Carb-1.11. Uronic acids

Monocarboxylic acids formally derived from aldoses by replacement of the CH₂OH group with a carboxy group are termed uronic acids (see 2-Carb-22).

2-Carb-1.12. Aldaric acids

The dicarboxylic acids formed from aldoses by replacement of both terminal groups (CHO and CH₂OH) by carboxy groups are called aldaric acids (see 2-Carb-23).

2-Carb-1.13. Glycosides

Glycosides are mixed acetals formally arising by elimination of water between the hemiacetal or hemiketal hydroxy group of a sugar and a hydroxy group of a second compound. The bond between the two components is called a glycosidic bond.

For an extension of this definition, see 2-Carb-33.

2-Carb-1.14. Oligosaccharides

Oligosaccharides are compounds in which monosaccharide units are joined by glycosidic linkages. According to the number of units, they are called disaccharides, trisaccharides, tetrasaccharides, pentasaccharides etc. The borderline with polysaccharides cannot be drawn strictly; however the term 'oligosaccharide' is commonly used to refer to a defined structure as opposed to a polymer of unspecified length or a homologous mixture. When the linkages are of other types, the compounds are regarded as oligosaccharide analogues. (See 2-Carb-37.)

Note. This definition is broader than that given in [6], to reflect current usage.

2-Carb-1.15. Polysaccharides

'Polysaccharide' (glycan) is the name given to a macromolecule consisting of a large number of monosaccharide (glycose) residues joined to each other by glycosidic linkages. The term poly(glycose) is not a full synonym for polysaccharide (glycan) (cf. [20]), because it includes macromolecules composed of glycose residues joined to each other by non-glycosidic linkages.

For polysaccharides containing a substantial proportion of amino sugar residues, the term polysaccharide is adequate, although the term glycosaminoglycan may be used where particular emphasis is desired.

Polysaccharides composed of only one kind of monosaccharide are described as homopolysaccharides (homoglycans). Similarly, if two or more different kinds of monomeric unit are present, the class name heteropolysaccharide (heteroglycan) may be used. (See 2-Carb-39.)

The term 'glycan' has also been used for the saccharide component of a glycoprotein, even though the chain length may not be large.

The term polysaccharide has also been widely used for macromolecules containing glycose or alditol residues in which both glycosidic and phosphate diester linkages are present.

2-Carb-1.16. Conventions for examples

1.16.1. Names of examples are given with an initial capital letter (e.g. 'L-glycero- β -D-gluco-Heptopyranose') to clarify the usage in headings and to show which letter controls the ordering in an alphabetical index.

1.16.2. The following abbreviations are commonly used for substituent groups in structural formulae: Ac (acetyl), Bn or PhCH₂ (benzyl), Bz or PhCO (benzoyl), Et (ethyl), Me (methyl), Me₃Si (not TMS) (trimethylsilyl), Bu^tMe₂Si (not TBDMS) (*tert*-butyldimethylsilyl), Ph (phenyl), Tf (triflyl = trifluoromethanesulfonyl), Ts (tosyl = toluene-*p*-sulfonyl), Tr (trityl).

2-Carb-2. Parent monosaccharides

2-Carb-2.1. Choice of parent structure

In cases where more than one monosaccharide structure is embedded in a larger molecule, a parent structure is chosen on the basis of the following criteria, applied in the order given until a decision is reached:

2.1.1. The parent that includes the functional group most preferred by general principles of organic nomenclature [13,14]. If there is a choice, it is made on the basis of the greatest number of occurrences of the most preferred functional group. Thus aldaric acid > uronic acid/ketoaldonic acid/aldonic acid > dialdose > ketoaldose/aldose > diketose > ketose.

2.1.2. The parent with the greatest number of carbon atoms in the chain, e.g. a heptose rather than a hexose.

2.1.3. The parent with the name that comes first in an alphabetical listing based on:

2.1.3.1. the trivial name or the configurational prefix(es) of the systematic name, e.g. allose rather than glucose, a *gluco* rather than a *gulo* derivative;

2.1.3.2. the configurational symbol D rather than L ;

2.1.3.3. the anomeric symbol α rather than β .

2.1.4. The parent with the most substituents cited as prefixes (bridging substitution, e.g. 2,3-*O*-methylene, is regarded as multiple substitution for this purpose).

2.1.5. The parent with the lowest locants (see [14], p. 17) for substituent prefixes.

2.1.6. The parent with the lowest locant for the first-cited substituent.

The implications of these recommendations for branched-chain structures are exemplified in 2-Carb-18.

Note 1. To maintain homomorphic relationships between classes of sugars, the (potential) aldehyde group of a uronic acid is regarded as the principal function for numbering and naming (see 2-Carb-2.2.1 and 2-Carb-22).

Note 2. To maintain integrity of carbohydrate names, it is sometimes helpful to overstep the strict order of principal group preference specified in general organic nomenclature [13,14]. For example, a carboxymethyl-substituted sugar can be named as such, rather than as an acetic acid derivative (see 2-Carb-31.2).

2-Carb-2.2. Numbering and naming the parent structure

The basis for the name is the structure of the parent monosaccharide in the acyclic form. Charts I and IV (2-Carb-10) give trivial names for parent aldoses and ketoses with up to six carbon atoms. 2-Carb-8.2 and 2-Carb-10.3 describe systematic naming procedures.

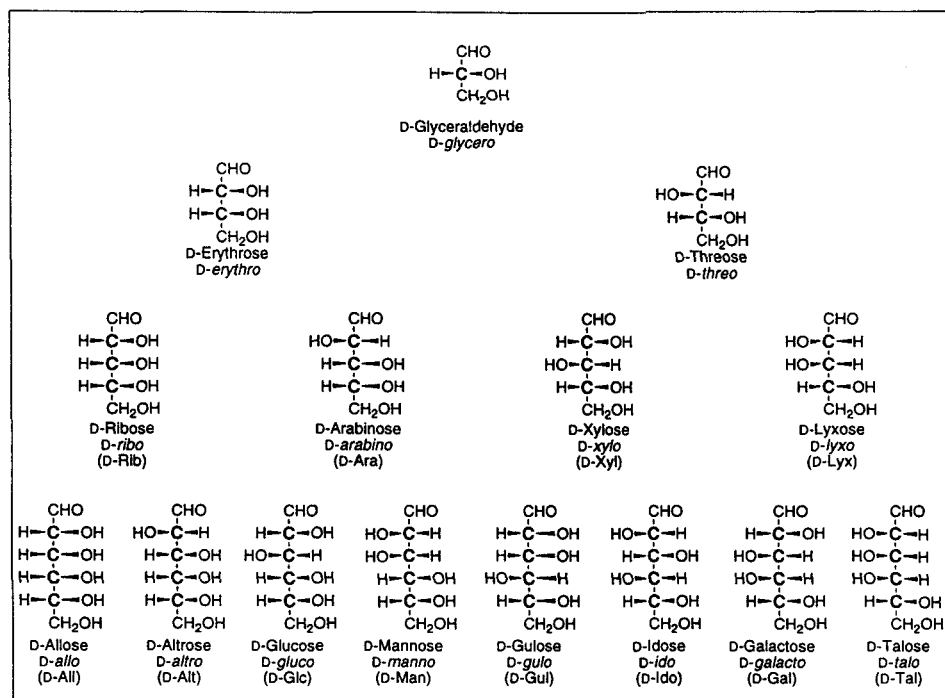


Chart I. Trivial names (with recommended three-letter abbreviations in parentheses) and structures (in the aldehydic, acyclic form) of the aldoses with three to six carbon atoms. Only the D-forms are shown; the L-forms are the mirror images. The chains of chiral atoms delineated in bold face correspond to the configurational prefixes given in italics below the names

2.2.1. Numbering

The carbon atoms of a monosaccharide are numbered consecutively in such a way that:

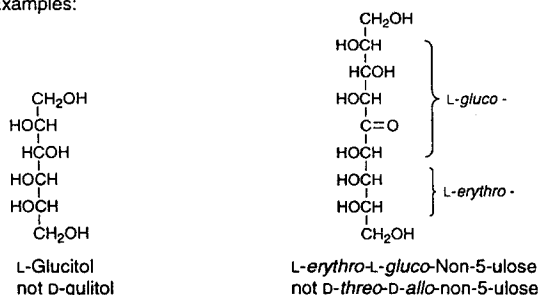
2.2.1.1. A (potential) aldehyde group receives the locant 1 (even if a senior function is present, as in uronic acids; see 2-Carb-2.1, note 1);

2.2.1.2. The most senior of other functional groups expressed in the suffix receives the lowest possible locant, i.e. carboxylic acid (derivatives) > (potential) ketonic carbonyl groups.

2.2.2. Choice of parent name

The name selected is that which comes first in the alphabet (configurational prefixes included). Trivial names are preferred for parent monosaccharides and for those derivatives where all stereocentres are stereochemically unmodified.

Examples:

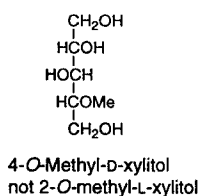


2.2.3. Choice between alternative names for substituted derivatives

When the parent structure is symmetrical, preference between alternative names for derivatives should be given according to the following criteria, taken in order:

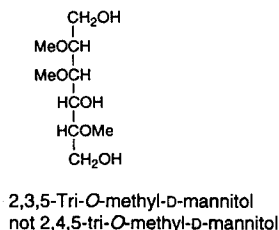
2.2.3.1. The name including the configurational symbol D rather than L.

Example:



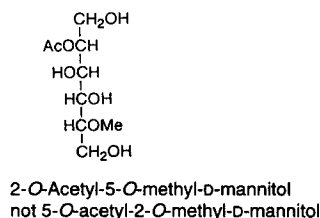
2.2.3.2. The name that gives the lowest set of locants (see [14], p. 17) to the substituents present.

Example:



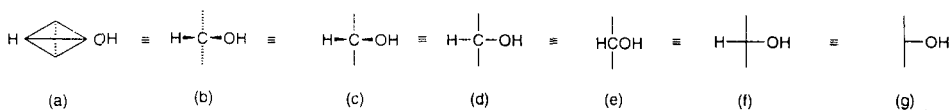
2.2.3.3. The name that, when the substituents have been placed in alphabetical order, possesses the lowest locant for the first-cited substituent.

Example:



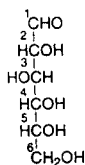
2-Carb-3. The Fischer projection of the acyclic form

In this representation of a monosaccharide, the carbon chain is written vertically, with the lowest numbered carbon atom at the top. To define the stereochemistry, each carbon atom is considered in turn and placed in the plane of the paper. Neighbouring carbon atoms are below, and the H and OH groups above the plane of the paper (see below).



Conventional representation of a carbon atom (e.g. C-2 of D-glucose) in the Fischer projection.
Representation (e) will be used in general in the present document.

The formula below is the Fischer projection for the acyclic form of D-glucose. The Fischer projections of the other aldoses (in the acyclic form) are given in Chart I (2-Carb-2.2).



D-Glucose

Note. The Fischer projection is not intended to be a true representation of conformation.

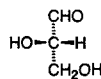
2-Carb-4. Configurational symbols and prefixes

2-Carb-4.1. Use of D and L

The simplest aldose is glyceraldehyde (occasionally called glycerol [21]). It contains one centre of chirality (asymmetric carbon atom) and occurs therefore in two enantiomeric forms, called D-glyceraldehyde and L-glyceraldehyde; these are represented by the projection formulae given below. It is known that these projections correspond to the absolute configurations. The configurational symbols D and L should appear in print in small-capital roman letters (indicated in typescript by double underlining> and are linked by a hyphen to the name of the sugar.



D-Glyceraldehyde

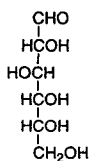


L-Glyceraldehyde

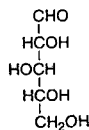
2-Carb-4.2. The configurational atom

A monosaccharide is assigned to the D or the L series according to the configuration at the highest-numbered centre of chirality. This asymmetrically substituted carbon atom is called the 'configurational atom'. Thus if the hydroxy group (or the oxygen bridge of the ring form; see 2-Carb-6) projects to the right in the Fischer projection, the sugar belongs to the D series and receives the prefix D-.

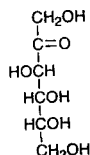
Examples:



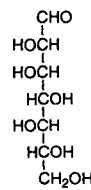
D-Glucose



D-Xylose

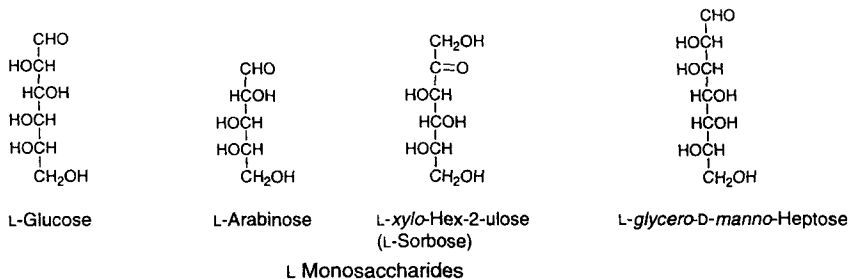


D-arabino-Hex-2-ulose
(D-Fructose)



D-glycero-L-gulo-Heptose

D Monosaccharides



2-Carb-4.3. Configurational prefixes in systematic names

In the systematic names of sugars or their derivatives, it is necessary to specify not only the configuration of the configurational atom but also the configurations of all CHOH groups. This is done by the appropriate configurational prefix. These prefixes are derived from the trivial names of the aldoses in Chart I (relevant portions of the structures are delineated in bold face). In monosaccharides with more than four asymmetrically substituted carbon atoms, where more than one configurational prefix is employed (see 2-Carb-8.3), each group of asymmetrically substituted atoms represented by a particular prefix has its own configurational symbol, specifying the configuration (D or L) of the highest numbered atom of the group.

The configurational prefixes are printed in lower-case italic (indicated in typescript by underlining), and are preceded by either D- or L-, as appropriate. For examples see 2-Carb-4.2 and 2-Carb-6.2

Note. In cyclic forms of sugars, the configuration at the anomeric chiral centre is defined in relation to the 'anomeric reference atom' (see 2-Carb-6.2).

2-Carb-4.4. Racemates and *meso* forms

Racemates may be indicated by the prefix DL-. Structures that have a plane of symmetry and are therefore optically inactive (e.g. erythritol, galactitol) are called *meso* forms and may be given the prefix '*meso*'.

2-Carb-4.5. Optical rotation

If the sign of the optical rotation under specified conditions is to be indicated, this is done by adding (+)- or (-)- before the configurational prefix. Racemic forms are indicated by (±)-.

Examples:

D-Glucose or (+)-D-glucose

D-Fructose or (-)-D-fructose

DL-Glucose or (±)-glucose

2-Carb-5. Cyclic forms and their representation

2-Carb-5.1. Ring size

Most monosaccharides exist as cyclic hemiacetals or hemiketals. Cyclic forms with a three-membered ring are called oxiroses, those with a four-membered ring oxetoses, those with a five-membered ring furanoses, with a six-membered ring pyranoses, with a seven-membered ring septanoses, with an eight-membered ring octanoses, and so on. To avoid ambiguities, the locants of the positions of ring closure may be given; the locant of the carbonyl group is always cited first, that of the hydroxy group second (for relevant examples of this see 2-Carb-6.4). Lack of ring size specification has no particular implication.

Note. The 'o' of oxirose, oxetose, and octanose is not elided after a prefix ending in 'o'.

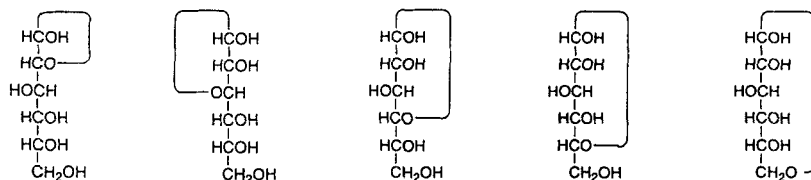
Example:

Nonooctanose, not nonooctanose.

If it is to be stressed that an open-chain form of an aldose is under consideration, the prefix '*aldehydo*' may be used. For ketoses, the prefix is '*keto*'.

2-Carb-5.2. The Fischer projection

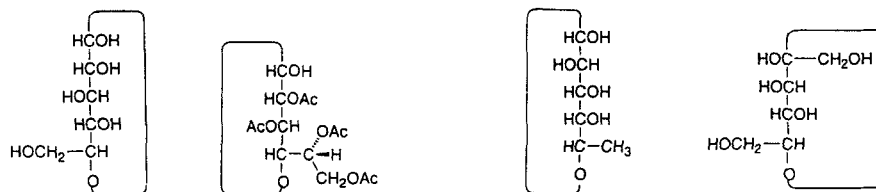
If a cyclic form of a sugar is to be represented in the Fischer projection, a long bond can be drawn between the oxygen involved in ring formation and the (anomeric) carbon atom to which it is linked, as shown in the following formulae for cyclic forms of α -D-glucose (see 2-Carb-6 for the meaning of α and β):



α -D-Glucosirose α -D-Glucosetose α -D-Glucufuranose α -D-Glucopyranose α -D-Glucoseptanose

2-Carb-5.3. Modified Fischer projection

To clarify steric relationships in cyclic forms, a modified Fischer projection may be used. The carbon atom bearing the ring-forming hydroxy group, $C-n$ ($C-5$ for glucopyranose) is rotated about its bond to $C-(n-1)$ ($C-4$ for glucopyranose) in order to bring all ring atoms (including the oxygen) into the same vertical line. The oxygen bridge is then represented by a long bond; it is imagined as being behind the plane of the paper. Examples are given below.



α -D-Glucopyranose

2,3,5,6-Tetra-O-acetyl- α -D-galactofuranose

β -L-Fucopyranose

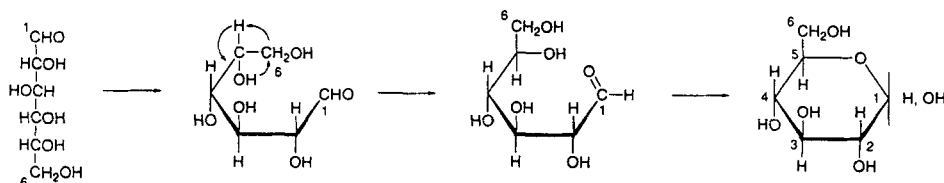
β -D-Fructofuranose

Thus the *trans* relationship between the hydroxymethyl group and the C-1 hydroxy group in α -D-glucopyranose, and the *cis* relationship between the methyl group and the C-1 hydroxy group in β -L-fucopyranose, are clearly shown. Note that representation of ketoses may require a different modification of the Fischer projection, as shown in the fructofuranose example above. Here C-2 is rotated about the bond with C-3 to accommodate the long bond to C-2 from the oxygen at C-5.

2-Carb-5.4 The Haworth representation

This is a perspective drawing of a simplified model. The ring is orientated almost perpendicular to the plane of the paper, but viewed from slightly above so that the edge closer to the viewer is drawn below the more distant edge, with the oxygen behind and C-1 at the right-hand end. To define the perspective, the ring bonds closer to the viewer are often thickened.

The following schematic representation of pyranose ring closure in D-glucose shows the reorientation at C-5 necessary to allow ring formation; this process corresponds to the change from Fischer to modified Fischer projection.



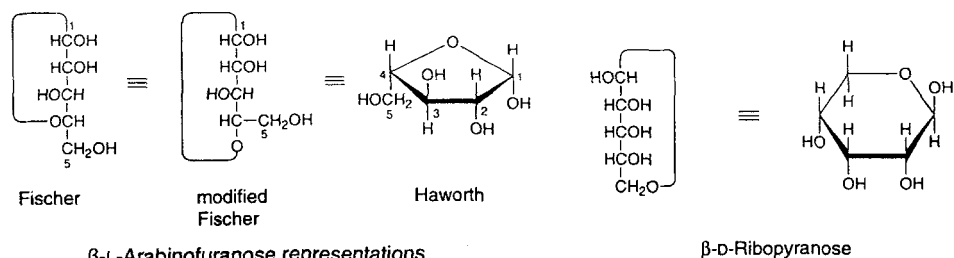
Haworth representation of D-glucopyranose

The orientation of the model described above results in a clockwise numbering of the ring atoms. Groups that appear to the right of the modified Fischer projection appear below the plane of the ring; those on the left

appear above. In the common Haworth representation of the pyranose form of D-aldohexoses, C-6 is above the plane.

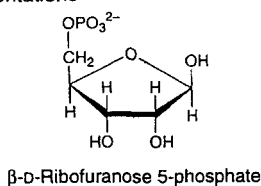
Generally, the configuration at the centre that yields the ring oxygen determines whether the rest of the carbon chain is below or above the plane of the ring.

Examples (for the use of α and β see 2-Carb-6):

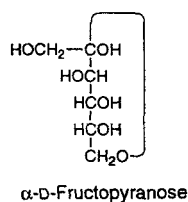


β -L-Arabinofuranose representations

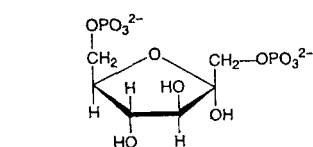
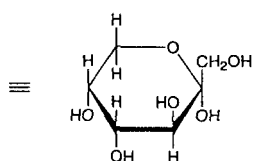
β -D-Ribopyranose



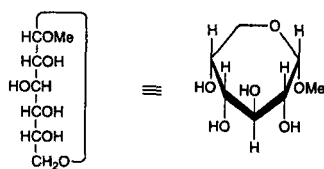
β -D-Ribofuranose 5-phosphate



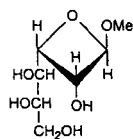
α -D-Fructopyranose



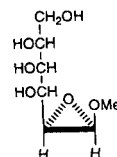
α -D-Fructofuranose 1,6-bisphosphate



Methyl α -D-glucoseptanoside



Methyl α -L-altrooxetoside



Methyl β -D-allooxiroside

Note. In writing Haworth formulae, the H atoms bound to the carbon atoms of the ring are often omitted to avoid crowding of the lettering in the ring. For the sake of clarity, the form with H atoms included is preferred in this document.

2-Carb-5.5. Unconventional Haworth representations

It is sometimes desirable to draw Haworth formulae with the ring in other orientations (see Chart II), when there are bulky substituents to be represented, or when linkages in oligo- or poly-saccharides are to be shown. If the ring is inverted [as in (g)-(1)], the numbering runs counterclockwise.

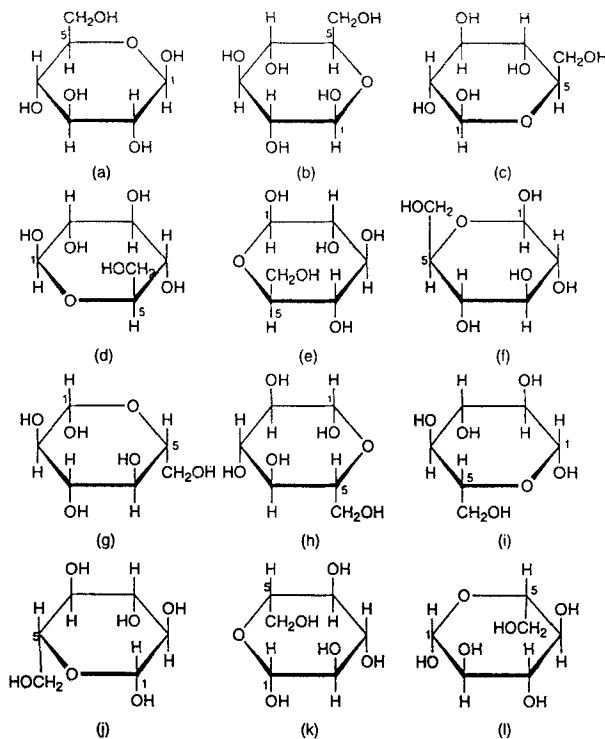
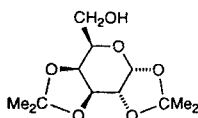


Chart II. β -D-Glucopyranose in the twelve possible Haworth representations (the hydrogen atoms are frequently omitted)

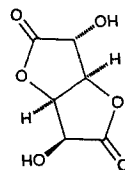
2-Carb-5.6. The Mills depiction

In some cases, particularly where additional rings are present, structural formulae can be clarified by use of the Mills depiction. Here the main hemiacetal ring is drawn in the plane of the paper; dashed bonds denote substituents below this plane, and thickened bonds those above.

Examples:



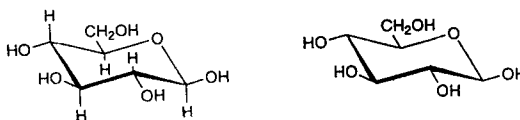
1,2:3,4-Di-O-isopropylidene- α -D-galactopyranose



D-Glucaro-1,4:6,3-dilactone

2-Carb-5.7. Depiction of conformation

The Haworth representation implies a planar ring. However, monosaccharides assume conformations that are not planar: these may be represented by Haworth conformational formulae. The nomenclature of conformations is described in 2-Carb-7. For example, β -D-glucopyranose assumes a chair conformation:

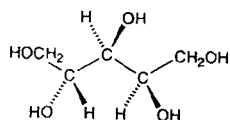


β -D-Glucopyranose in a chair conformation

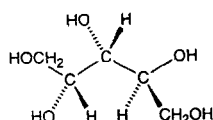
Note. The hydrogen atoms bonded to carbon are frequently omitted, but their inclusion may be necessary to make a stereochemical point.

2-Carb-5.8. Conformations of acyclic chains

Conformational depictions of acyclic sugar chains are conveniently expressed by locating certain atoms in the plane of the paper and orientating the remaining atoms or groups appropriately above and below that plane, as shown for D-arabinitol and xylitol (it should be recognized that the favoured conformation does not necessarily have all the carbon atoms in the same plane):



D-Arabinitol



Xylitol

2-Carb-6. Anomeric forms; use of α and β

2-Carb-6.1. The anomeric centre

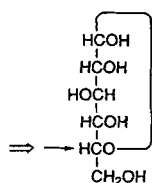
The new centre of chirality generated by hemiacetal ring closure is called the anomeric centre. The two stereoisomers are referred to as anomers, designated α or β according to the configurational relationship between the anomeric centre and a specified anomeric reference atom.

2-Carb-6.2. The anomeric reference atom and the anomeric configurational symbol (α or β)

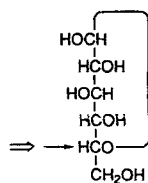
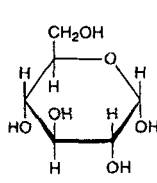
The anomeric reference atom is the configurational atom (see 2-Carb-4.2 and 4.3) of the parent, unless multiple configurational prefixes (see 2-Carb-8.3) are used. If multiple configurational prefixes are used, the anomeric reference atom is the highest-numbered atom of the group of chiral centres next to the anomeric centre that is involved in the heterocyclic ring and specified by a single configurational prefix. In the α anomer, the exocyclic oxygen atom at the anomeric centre is formally *cis*, in the Fischer projection, to the oxygen attached to the anomeric reference atom; in the β anomer these oxygen atoms are formally *trans*.

The anomeric symbol α or β , followed by a hyphen, is placed immediately before the configurational symbol D or L of the trivial name or of the configurational prefix denoting the group of chiral carbon atoms that includes the anomeric reference atom.

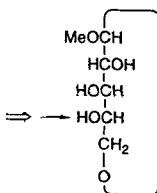
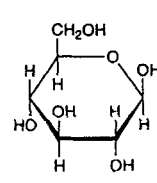
Examples:

 α -D-glucopyranose

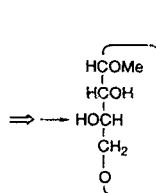
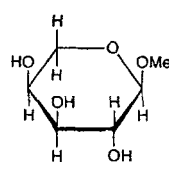
≡

 β -D-glucopyranose

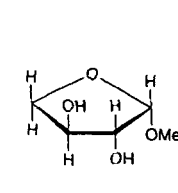
≡

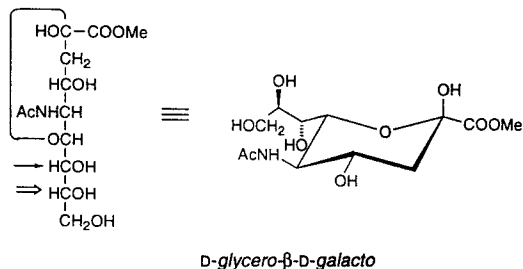
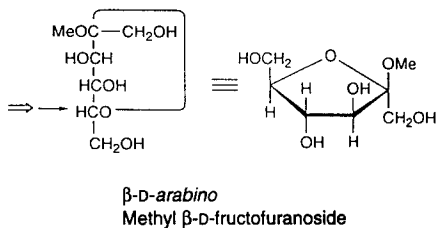
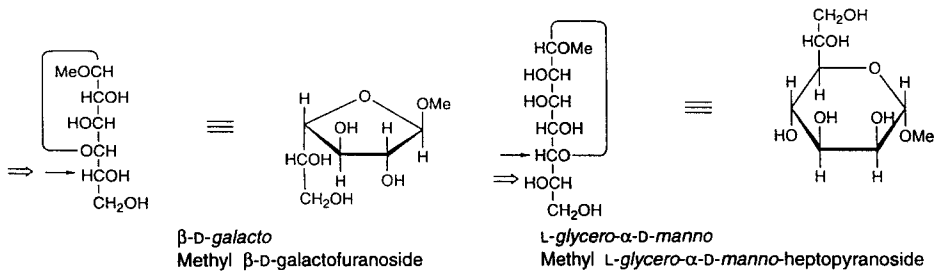
 α -L-arabinopyranoside

≡

 β -L-threofuranoside

≡





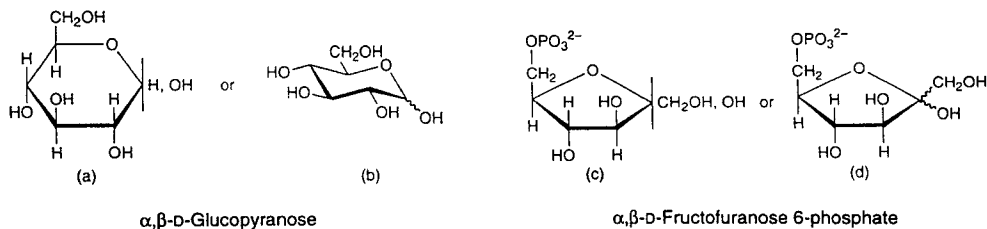
\rightarrow denotes the anomeric reference atom; \Rightarrow denotes the configurational atom.

Note. For simple aldoses up to aldohexoses, and ketoses up to hept-2-uloses, the anomeric reference atom and the configurational atom are the same.

2-Carb-6.3. Mixtures of anomers

In solution, most simple sugars and many of their derivatives occur as equilibrium mixtures of tautomers. The presence of a mixture of two anomers of the same ring size may be indicated in the name by the notation α,β -, e.g. α,β -D-glucose. In formulae, the same situation can be expressed by separating the representation of the ligands at the anomeric centre from the α and β bonds [see examples (a) and (c)], or by use of a wavy line [(b) and (d)] (particularly if hydrogen atoms are omitted).

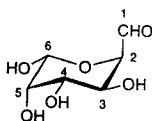
Examples:



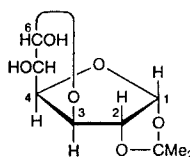
2-Carb-6.4. Use of α and β

The Greek letters α and β are applicable only when the anomeric carbon atom has a lower locant than the anomeric reference atom. In the case of dialdoses (cf. 2-Carb-9), some diketoses (cf. 2-Carb-11) and aldoketoses (cf. 2-Carb-12), ring closure is also possible in the other direction, i.e. of a carbonyl group with a higher locant than the reference carbon atom with a hydroxy group having a lower locant. In this case, the configuration of the anomeric carbon atom is indicated by the appropriate symbol R or S according to the sequence rule (cf. Section E in [13]).

Examples:



(6*R*)-D-*gluco*-Hexodialdo-6,2-pyranose



(6*S*)-1,2-*O*-Isopropylidene- α -D-*gluco*-hexodialdo-1,4,6,3-difuranose

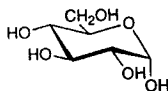
Note that locant numerals (potential carbonyl first) may be needed before the ring-size suffix in such cases.

2-Carb-7. Conformation of cyclic forms*

2-Carb-7.1. The conformational descriptor

The conformation, i.e. the (approximate) spatial arrangement of the ring atoms of a monosaccharide in the cyclic form, may be indicated by an italic capital letter designating the type of ring shape, and numerals, distinguishing the variants. The conformational descriptor is joined to the end of the name of the monosaccharide by a hyphen.

Example:

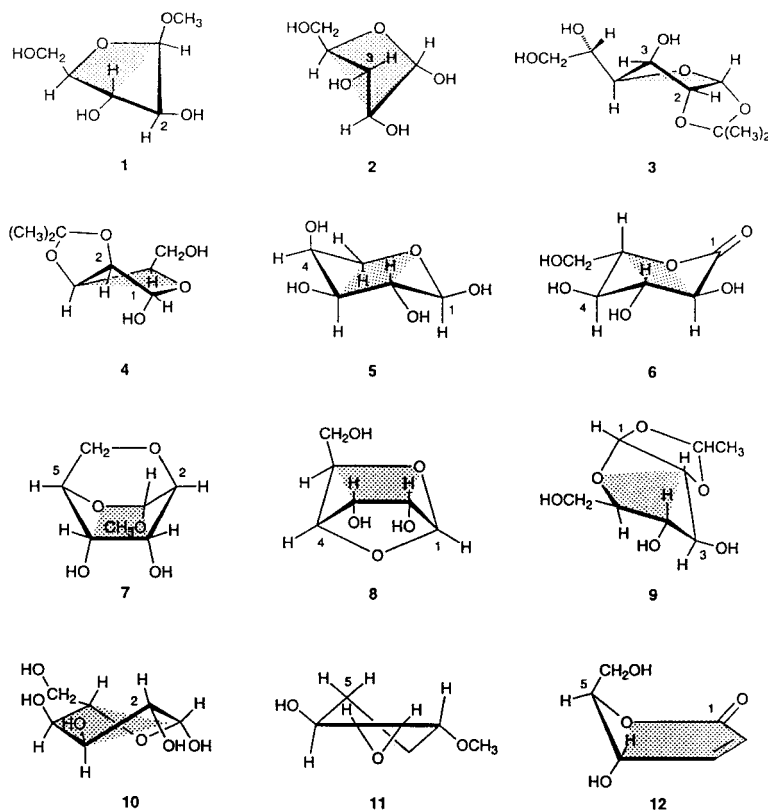


α -D-Glucopyranose-⁴C₁

Table 1. Conformations and their notations; some examples are shown in Chart III

Type of sugar	Conformation	Atoms of reference plane	Above plane	Below plane	Notation	Example
Aldofuranose	envelope	O-4,C-1,C-3,C-4	-	C-2	² E ₂	1
Aldofuranose	envelope	C-1,C-2,C-4,O-4	C-3	-	³ E	2
Aldofuranose	twist	C-1,O-4,C-4	C-3	C-2	³ T ₂	3
Aldofuranose	twist	C-3,C-4,O-4	C-2	C-1	² T ₁	4
Aldopyranose	chair	C-2,C-3,C-5,O-5	C-4	C-1	⁴ C ₁	5
Pyranoid lactone	chair	C-2,C-3,C-5,O-5	C-1	C-4	¹ C ₄	6
Aldopyranose	boat	O-5,C-1,C-3,C-4	C-2,C-5	-	^{2,5} B	7
Aldopyranose	boat	C-2,C-3,C-5,O-5	-	C-1,C-4	^B _{1,4}	8
Aldopyranose	skew	C-2,C-4,C-5,O-5	C-1	C-3	¹ S ₃	9
Aldopyranose	skew	C-1,C-3,C-4,C-5	C-2	O-5	² S _O	10
Aldopyranose	half-chair	C-1,C-2,C-3,C-4	C-5	S-5	⁵ H _S	11
Pyranoid lactone	envelope	C-1,C-2,C-3,C-4,O-5	C-5	-	⁵ E	12

* This is an abridged version of the document 'Conformational Nomenclature for Five- and Six-membered Ring Forms of Monosaccharides and their Derivatives. Recommendations 1980 [3].



- | | | | |
|---|--|---|--|
| 1 | Methyl β -D-arabinofuranoside- E_2 | 2 | α -D-Arabinofuranose- 3E |
| 3 | 1,2- <i>O</i> -Isopropylidene- β -L-idofuranose- 2T_1 | 4 | 2,3- <i>O</i> -Isopropylidene- α -D-lyxofuranose- 2T_1 |
| 5 | α -L-Arabinopyranose- 4C_1 | 6 | L-Glucono-1,5-lactone- 1C_4 |
| 7 | Methyl 2,6-anhydro- α -D-altropyranoside- $^{2.5}B$ | 8 | 1,4-Anhydro- α -D-allopyranose- $B_{1,4}$ |
| 9 | 1,2- <i>O</i> -Ethylidene- α -D-glucofuranose- 1S_3 | 10 | β -L-Altropyranose- 2S_0 |
| | 11 | Methyl 2,3-anhydro-5-thio- β -L-lyxopyranoside- 5H_5 | |
| | 12 | 2,3-Dideoxy-D-erythro-hex-2-enono-1,5-lactone- 5E | |

Chart III. Drawings of the conformations listed in Table 1. The reference plane is stippled.

2-Carb-7.2. Notation of ring shape

The appropriate letters are as follows. Five-membered rings: *E* for envelope and *T* for twist; six-membered rings: *C* for chair, *B* for boat, *S* for skew, *H* for half-chair, and *E* for envelope. Examples are given in Chart III.

2-Carb-7.3. Notation of variants

The variants are distinguished by the locants of those ring atoms that lie outside a reference plane (defined below) and are listed for some examples in Table 1. The locants of ring atoms that lie on the side of the reference plane from which numbering appears clockwise (i.e. the upper side in the normal Haworth representation of furanoses and pyranoses) are written as superscripts and precede the letter; those that lie on the other side are written as subscripts and follow the letter. Heteroatoms (e.g. O, S) are indicated by their subscript or superscript atomic symbols. Table 1 gives the notations and Chart III some examples.

Six-membered rings

Chairs. The reference plane is defined by two parallel ring sides, so chosen that the lowest-numbered carbon atom in the ring is exoplanar (examples 5 and 6).

Boats. The reference plane is defined by the two parallel 'sides' of the boat (examples 7 and 8).

Skews. Each skew form has two potential reference planes, containing three adjacent atoms and the remaining non-adjacent atom. The reference plane is so chosen that the lowest-numbered carbon atom in the ring, or the atom numbered next above it, is exoplanar, in that order of preference (examples 9 and 10).

Half-chairs. The reference plane is defined by the four adjacent coplanar atoms (example 11).

Envelopes. The reference plane is defined by the five adjacent coplanar atoms (example 12).

Five-membered rings

Envelopes. The reference plane is defined by the four adjacent coplanar atoms (examples 1 and 2).

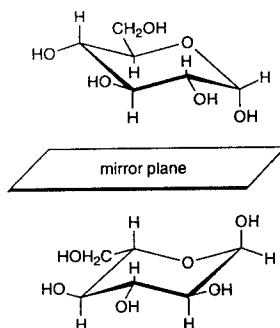
Twists. The reference plane is defined by three adjacent ring-atoms, so chosen that the exoplanar atoms lie on opposite sides of the plane (examples 3 and 4).

Note 1. Many of the possible conformations are not likely to contribute significantly to the chemistry of a particular monosaccharide, but must be stabilized by formation of additional rings, as in anhydrides or other derivatives. Some others may occur as transition-state intermediates.

Note 2. A more precise specification of conformation can be achieved by use of the Cremer-Pople puckering parameters [22].

2-Carb-7.4. Enantiomers

The conformational symbols for enantiomers are different. It is therefore important to state in the context whether the D or the L form is under consideration. Enantiomers have the same reference plane (see 2-Carb-7.3), and it should be noted that the mirror image of α -D-glucose-⁴C₁ is α -L-glucose-¹C₄.



Mirror images: α -D-glucopyranose-⁴C₁ (upper) and α -L-glucopyranose-¹C₄ (lower)

2-Carb-8. Aldoses**2-Carb-8.1. Trivial names**

The aldoses with three to six carbon atoms have trivial names which are given, together with the formulae in the Fischer projection, in Chart I (2-Carb-2.2). (See also the alphabetical listing of trivial names in the Appendix.)

The trivial names form the basis of the configurational prefixes (see 2-Carb-4.3).

2-Carb-8.2. Systematic names

Systematic names are formed from a stem name and a configurational prefix or prefixes. The stem names for the aldoses with three to ten carbon atoms are triose, tetrose, pentose, hexose, heptose, octose, nonose, decose. The chain is numbered so that the carbonyl group is at position 1.

The configuration of the CHOH groups of the sugar is designated by the appropriate configurational prefix(es) from Chart I. When used in systematic names, these prefixes are always to be in lower case letters (with no initial capital), and italicized in print. Each prefix is qualified by D or L (Chart I shows only the D structures).

Examples:

D-ribo-Pentose for *D*-ribose

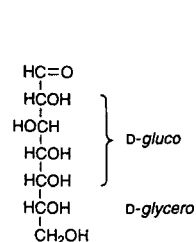
D-manno-Hexose for *D*-mannose.

The trivial names are preferred for the parent sugars and for those derivatives where all stereocentres are unmodified.

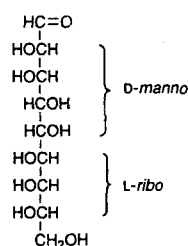
2-Carb-8.3. Multiple configurational prefixes

An aldose containing more than four chiral centres is named by adding two or more configurational prefixes to the stem name. Prefixes are assigned in order to the chiral centres in groups of four, beginning with the group proximal to C-1. The prefix relating to the group of carbon atom(s) farthest from C-1 (which may contain less than four atoms) is cited first.

Examples:



D-glycero-*D-gluco*-Heptose
not *D-gluco*-*D-glycero*-heptose

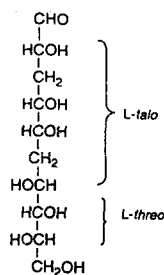


L-ribo-*D-manno*-Nonose
not *D-manno*-*L-ribo*-nonose

2-Carb-8.4. Multiple sets of chiral centres

If sequences of chiral centres are separated by non-chiral centres, the non-chiral centres are ignored, and the remaining set of chiral centres is assigned the appropriate configurational prefix (for four centres or less) or prefixes (for more than four centres).

Example:



3,5-Dideoxy-*L-threo*-*L-talo*-decose

Note 1. This convention is not needed for parent aldoses, only for deoxy aldoses, ketoses and similar compounds (see 2-Carb-10.4 and 2-Carb-11.2).

Note 2. Since all aldoses up to the hexoses have trivial names that are preferred, the systematic names apply only to the higher aldoses. However, the configurational prefixes are also used to name ketoses (see below) and other monosaccharides.

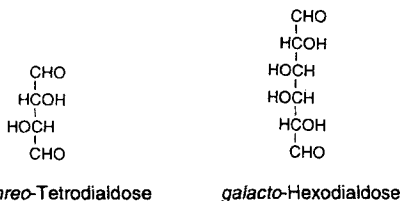
2-Carb-8.5. Anomeric configuration in cyclic forms

For the specification of α and β in cyclic forms see 2-Carb-6.

2-Carb-9. Dialdoses

Systematic names for individual dialdoses are formed from the systematic stem name for the corresponding aldose (see 2-Carb-8.2), but with the ending 'odialdose' instead of 'ose', and the appropriate configurational prefix (Chart I). A choice between the two possible aldose parent names is made on the basis of 2-Carb-2.2.2.

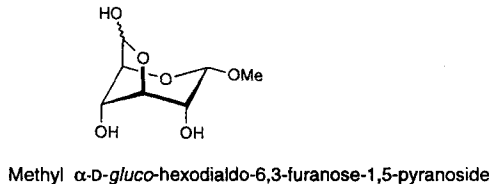
Examples:



Note. The prefix '*meso*' could be included in the latter case, but it is not needed to define the structure.

If a cyclic form is to be named, the locants of the anomeric centre and of the carbon atom bearing the ring oxygen atom must be given (in that order) (cf. 2-Carb-6.4). If there is more than one ring size designator, they are placed in alphabetical order (e.g. furanose before pyranose).

Examples:



2-Carb-10. Ketoses

2-Carb-10.1. Classification

Ketoses are classified as 2-ketoses, 3-ketoses, etc., according to the position of the (potential) carbonyl group. The locant 2 may be omitted if no ambiguity can arise, especially in a biochemical context.

2-Carb-10.2. Trivial names

Ketoses with three to six carbon atoms are shown in Chart IV, with trivial names (and three-letter abbreviations) in parentheses. (See also the alphabetical listing of trivial names in the Appendix.)

The trivial names 'D-erythrulose' for D-*glycero*-tetrulose, 'D-ribulose' for D-*erythro*-pent-2-ulose, and 'D-xylulose' for D-*threo*-pent-2-ulose contain stereochemical redundancy and should not be used for naming derivatives. Sedoheptulose is the accepted trivial name for D-*altro*-hept-2-ulose.

2-Carb-10.3. Systematic names

The systematic names are formed from the stem name and the appropriate configurational prefix.

The stem names are formed from the corresponding aldose stem names (2-Carb-8.2) by replacing the ending '-ose' with '-ulose', preceded by the locant of the carbonyl group, e.g. hex-3-ulose. The chain is numbered so that the carbonyl group receives the lowest possible locant. If the carbonyl group is in the middle of a chain with an odd number of carbon atoms, a choice between alternative names is made according to 2-Carb-2.2.2.

Note. In Chemical Abstracts Service (CAS) usage the locant for the carbonyl group precedes the stem name, e.g. 3-hexulose.

For examples see 2-Carb-10.4.

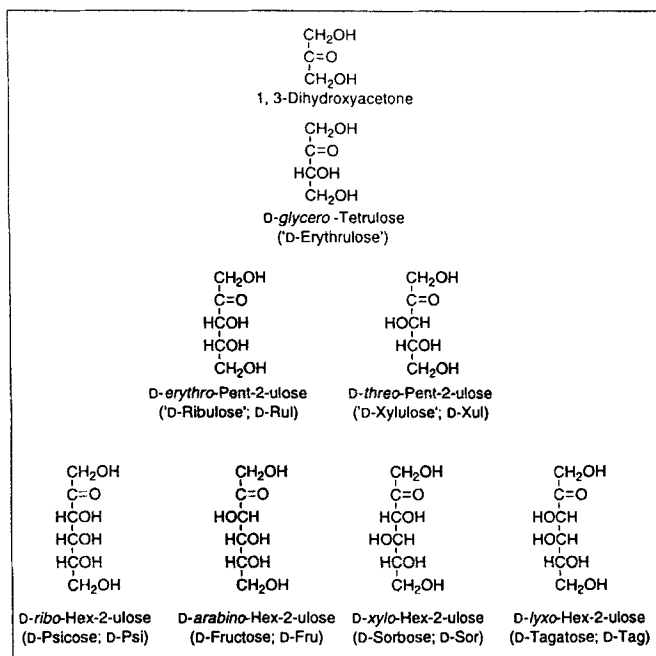
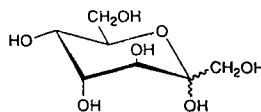
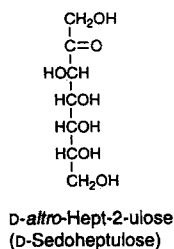
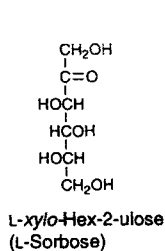


Chart IV. Structures, with systematic and trivial names, of the 2-ketoses with three to six carbon atoms

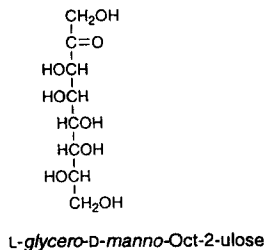
2-Carb-10.4. Configurational prefixes

For 2-ketoses, configurational prefixes are given in the same way as for aldoses (see 2-Carb-8.2 and 2-Carb-8.3).

Examples:

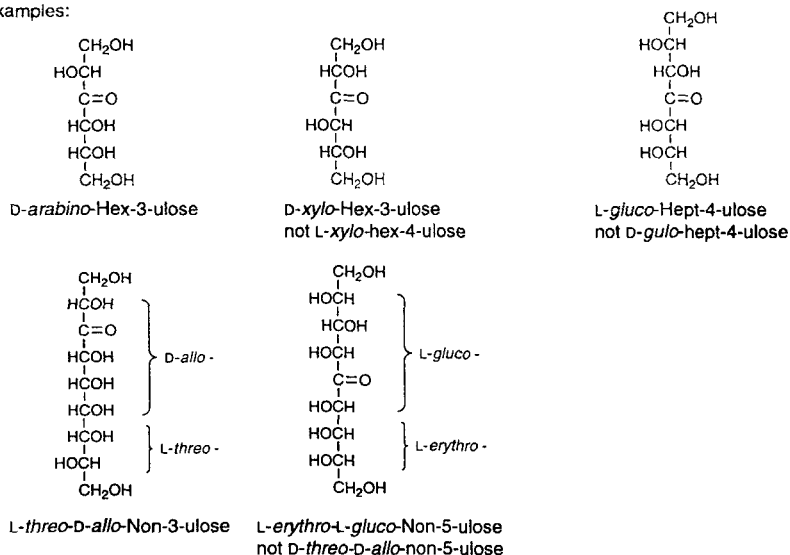


D-altr/o-Hept-2-ulopyranose



For ketoses with the carbonyl group at C-3 or a higher-numbered carbon atom, the carbonyl group is ignored and the set of chiral centres is given the appropriate prefix or prefixes according to Chart I (cf. 2-Carb-8.4).

Examples:

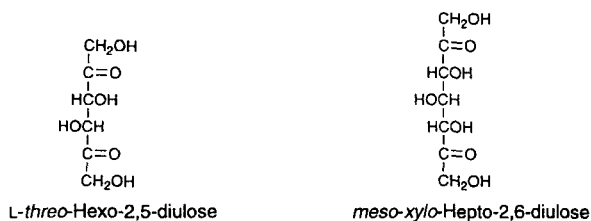


2-Carb-11. Diketoses

2-Carb-11.1. Systematic names

The systematic name of a diketose is formed by replacing the terminal '-se' of the stem name by '-diulose'. The locants of the (potential) carbonyl groups must be the lowest possible and appear before the ending. The stem name is preceded by the appropriate configurational prefix. If there is a choice of names, a decision is made on the basis of 2-Carb-2.2.2. In cyclic forms, locants may be needed for the positions of ring closure; that of the (potential) carbonyl group is cited first.

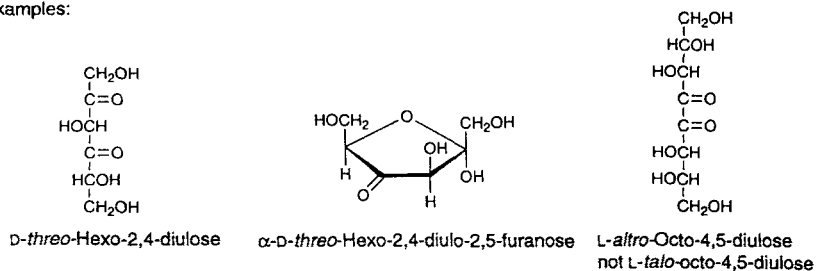
Examples:

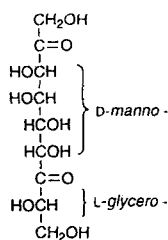


2-Carb-11.2. Multiple sets of chiral centres

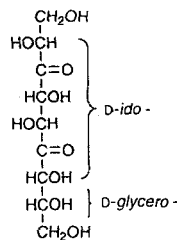
If the carbonyl group(s) divides the sequence of chiral centres, the configurational prefixes are assigned in the normal manner (see 2-Carb-8.4) for all chiral centres; the non-chiral centres are ignored.

Examples:





L-glycero-D-manno-Nono-2,7-diulose



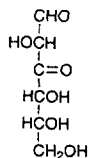
D-glycero-D-ido-Nono-3,6-diulose

2-Carb-12. Ketoaldoses (aldoketoses, aldoses)

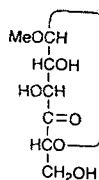
2-Carb-12.1. Systematic names

Names of ketoaldoses are formed in the same way as those of diketoses, but with use of the termination '-ulose' in place of the terminal '-e' of the corresponding aldose name (2-Carb-8.2). The carbon atom of the (potential) aldehydic carbonyl group is numbered 1, and this locant is not cited in the name. The locant of the (potential) ketonic carbonyl group is given (as an infix before '-ulose') unless it is 2; it may then be omitted (in this text, this locant is always retained for the sake of clarity). In cyclic forms, locants may be needed for the positions of ring closure; that of the (potential) carbonyl group is cited first. The position of the ring-size designator (e.g. pyrano) depends upon which carbonyl group is involved in ring formation (see examples).

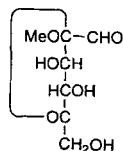
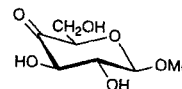
Examples:



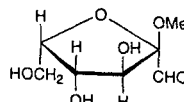
D-arabino-Hexos-3-ulose



Methyl β-D-xylo-hexopyranosid-4-ulose



Methyl α-L-xylo-Hexos-2-ulo-2,5-furanoside

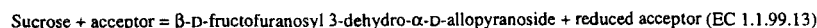
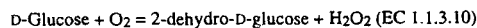


2-Carb-12.2. 'Dehydro' names

In a biochemical context, the naming of aldoketoses as 'dehydro' aldoses is widespread. Thus D-xylo-hexopyranos-4-ulose would be termed 4-dehydro-D-glucose. This usage of 'dehydro' can give rise to names which are stereochemically redundant, and should not be employed for naming derivatives.

Note. In Enzyme Nomenclature [23] dehydro names are used in the context of enzymic reactions. The substrate is regarded as the parent compound, but the name of the product is chosen according to the priority given in 2-Carb-2.2.

Examples:

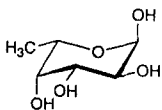


2-Carb-13. Deoxy sugars

2-Carb-13.1. Trivial names

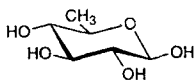
Several deoxy sugars have trivial names established by long usage, e.g. fucose (Fuc), quinovose (Qui) and rhamnose (Rha). They are illustrated here in the pyranose form. These names are retained for the unmodified sugars, but systematic names are usually preferred for the formation of names of derivatives, especially where deoxygenation is at a chiral centre of the parent sugar. (See also the alphabetical listing of trivial names in the Appendix.)

Examples:



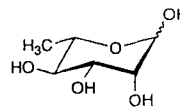
α -L-Fucopyranose

6-Deoxy- α -L-galactopyranose



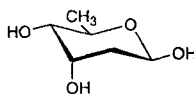
β -D-Quinovopyranose

6-Deoxy- β -D-glucopyranose

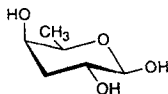


L-Rhamnopyranose

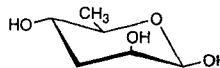
6-Deoxy-L-mannopyranose



2,6-Dideoxy- β -D-ribo-hexopyranose
(β -Digitoxopyranose)



3,6-Dideoxy- β -D-xylo-hexopyranose
(β -Abequopyranose)



3,6-Dideoxy- β -D-*arabino*-hexopyranose
(β -Tyvelopyranose)

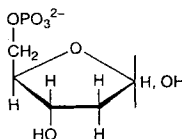
Other trivial names that have been used include ascarylose for 3,6-dideoxy-L-*arabino*-hexose, coltose for 3,6-dideoxy-L-*xylo*-hexose and paratose for 3,6-dideoxy-D-*ribo*-hexose.

Note. Sugars with a terminal CH_3 group should be named as ω -deoxy sugars, as shown above, not C-methyl derivatives.

2-Carb-13.2. Names derived from trivial names of sugars

Use of 'deoxy-' in combination with an established trivial name (see Charts I and II) is straightforward if the formal deoxygenation does not affect the configuration at any asymmetric centre. However if 'deoxy' removes a centre of chirality, the resulting names contain stereochemical redundancy. In such cases, systematic names are preferred, especially for the naming of derivatives.

Note. The names 2-deoxyribose (for 2-deoxy-D-*erythro*-pentose) and 2-deoxyglucose (for 2-deoxy-D-*arabino*-hexose) are often used.



2-Deoxy-D-*erythro*-pentofuranose 5-phosphate

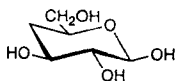
2-Carb-13.3. Systematic names

The systematic name consists of the prefix 'deoxy-', preceded by the locant and followed by the stem name with such configurational prefixes as necessary to describe the configuration(s) at the asymmetric centres

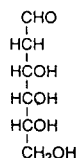
present in the deoxy compound. Configurational prefixes are cited in order commencing at the end farthest from C-1. 'Deoxy' is regarded as a detachable prefix, i.e. it is placed in alphabetical order with any substituent prefixes.

Note. The treatment of 'anhydro' (see 2-Carb-26), 'dehydro' (see 2-Carb-17.3) and 'deoxy' as detachable prefixes follows long-standing practice in carbohydrate chemistry, but is in conflict with [14] (p. 12).

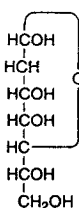
Examples:



4-Deoxy- β -D-xylo-hexopyranose
not 4-deoxy- β -D-galactopyranose

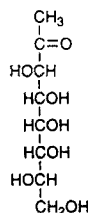
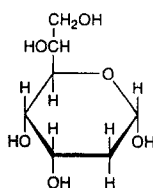


2-Deoxy-D-ribo-hexose not 2-deoxy-D-allose

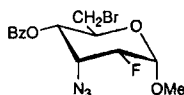


2-Deoxy- α -D-allo-heptopyranose

≡



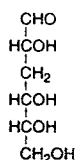
1-Deoxy-L-glycero-D-altro-oct-2-ulose



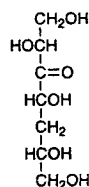
Methyl 3-azido-4-O-benzoyl-6-bromo-2,3,6-trideoxy-2-fluoro- α -D-allopyranoside

If the CH_2 group divides the chiral centres into two sets, it is ignored for the purpose of assigning a configurational prefix; the prefix(es) assigned should cover the entire sequence of chiral centres (see 2-Carb-8.4).

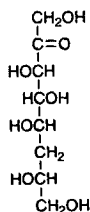
Examples:



3-Deoxy-D-ribo-hexose
not 3-deoxy-D-erythro-D-glycero-hexose



5-Deoxy-D-arabino-hept-3-ulose
not 5-deoxy-D-glycero-D-glycero-L-glycero-hept-3-ulose



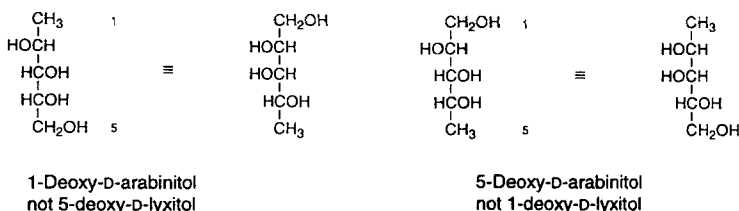
6-Deoxy-L-gluco-oct-2-ulose
not 6-deoxy-L-glycero-L-xylo-oct-2-ulose

If the anomeric hydroxy group is replaced by a hydrogen atom, the compound is named as an anhydro alditol (2-Carb-26).

2-Carb-13.4. Deoxy alditols

The name of an aldose derivative in which the aldehyde group has been replaced by a terminal CH₃ group is derived from that of the appropriate alditol (see 2-Carb-19) by use of the prefix 'deoxy-'.

Examples:



The alditols from fucose and rhamnose are frequently termed fucitol and rhamnitol (see 2-Carb-19.1).

2-Carb-14. Amino sugars

2-Carb-14.1. General principles

The replacement of an alcoholic hydroxy group of a monosaccharide or monosaccharide derivative by an amino group is envisaged as substitution of the appropriate hydrogen atom of the corresponding deoxy monosaccharide by the amino group. The stereochemistry at the carbon atom carrying the amino group is expressed according to 2-Carb-8.2, with the amino group regarded as equivalent to OH.

Some examples of *N*-substituted derivatives are given here; for a detailed treatment see 2-Carb-25.

2-Carb-14.2. Trivial names

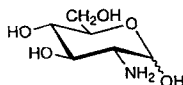
Accepted trivial names are as follows.

- D-Galactosamine for 2-amino-2-deoxy-D-galactose
- D-Glucosamine for 2-amino-2-deoxy-D-glucose
- D-Mannosamine for 2-amino-2-deoxy-D-mannose
- D-Fucosamine for 2-amino-2,6-dideoxy-D-galactose
- D-Quinovosamine for 2-amino-2,6-dideoxy-D-glucose
- Neuraminic acid for 5-amino-3,5-dideoxy-D-glycero-D-galacto-non-2-ulosonic acid
- Muramic acid for 2-amino-3-*O*-[(*R*)-1-carboxyethyl]-2-deoxy-D-glucose.

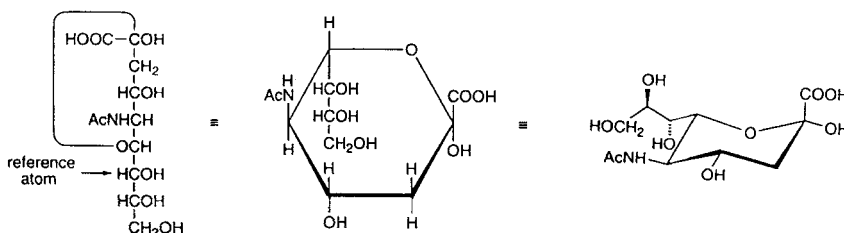
In the last two cases the trivial name refers specifically to the D enantiomer. (See also the alphabetical listing of trivial names in the Appendix.)

Such names as 'bacillosamine' for 2,4-diamino-2,4,6-trideoxy-D-glucose and 'garosamine' for 3-deoxy-4-*C*-methyl-3-methylamino-*L*-arabinose are not recommended, as they imply replacement of OH by NH₂ in a nonexistent parent sugar.

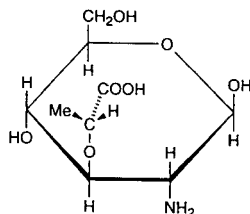
Examples:



2-Amino-2-deoxy-D-glucopyranose (D-glucosamine).



5-Acetamido-3,5-dideoxy-D-glycero- α -D-galacto-non-2-ulopyranosonic acid (*N*-acetyl- α -neuraminic acid, α -Neu5Ac), drawn in three ways (note that C-7 is the anomeric reference atom)



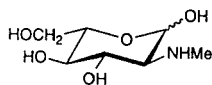
2-Amino-3-*O*-[(*R*)-1-carboxyethyl]-2-deoxy- β -D-glucopyranose (β -muramic acid)

For examples with nitrogen in the ring, see 2-Carb-34.1.

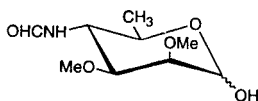
2-Carb-14.3. Systematic names

The compounds are named by use of a combination of 'deoxy-' and 'amino-' prefixes. When the complete name of the derivative includes other prefixes, 'deoxy-' takes its place in the alphabetical order of detachable prefixes.

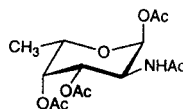
Examples:



2-Deoxy-2-methylamino-L-glucopyranose



4,6-Dideoxy-4-formamido-2,3-di-*O*-methyl-D-mannopyranose



2-Acetamido-1,3,4-tri-*O*-acetyl-2,6-dideoxy- α -L-galactopyranose

When the amino group is at the anomeric position, the compound is normally named as a glycosylamine (see 2-Carb-33.6).

2-Carb-15. Thio sugars and other chalcogen analogues

Replacement of a hydroxy oxygen atom of an aldose or ketose, or of the oxygen atom of the carbonyl group of the acyclic form of an aldose or ketose, by sulfur is indicated by placing the prefix 'thio', preceded by the appropriate locant, before the systematic or trivial name of the aldose or ketose.

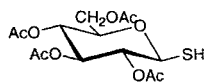
Replacement of the ring oxygen atom of the cyclic form of an aldose or ketose by sulfur is indicated in the same way, the number of the non-anomeric adjacent carbon atom of the ring being used as locant.

Selenium and tellurium compounds are named likewise, by use of the prefix 'seleno' or 'telluro'.

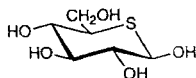
Sulfoxides (or selenoxides or telluroxides) and sulfones (or selenones or tellurones) may be named by functional class nomenclature [13].

Note. The appropriate prefix is thio, not thia; the latter is used in systematic organic chemical nomenclature to indicate replacement of CH₂ by S.

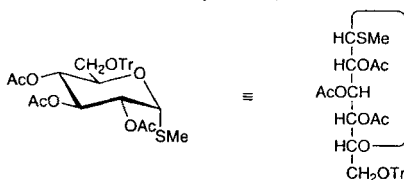
Examples:



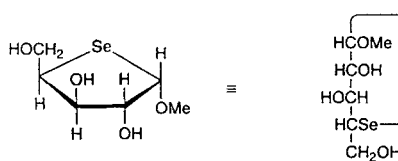
2,3,4,6-Tetra-*O*-acetyl-1-thio- β -D-glucopyranose



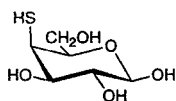
5-Thio- β -D-glucopyranose



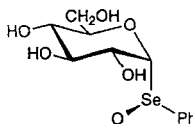
Methyl 2,3,4-tri-*O*-acetyl-1-thio-6-*O*-trityl- α -D-glucopyranoside



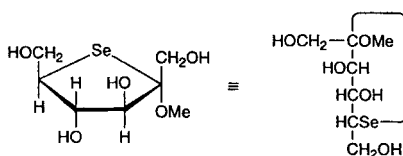
Methyl 4-seleno- α -D-xylofuranoside



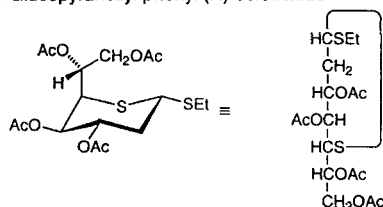
4-Thio- β -D-galactopyranose



α -D-Glucopyranosyl phenyl (*R*)-selenoxide



Methyl 5-seleno- α -D-fructofuranoside



Ethyl 3,4,6,7-tetra-*O*-acetyl-2-deoxy-1,5-dithio- α -D-*gluco*-heptopyranoside

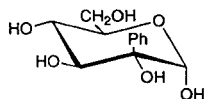
Note. It is common practice in carbohydrate names to regard 'thio' as detachable, and therefore alphabetized with any other prefixes.

2-Carb-16. Other substituted monosaccharides

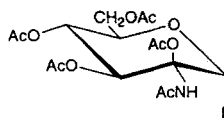
2-Carb-16.1. Replacement of hydrogen at a non-terminal carbon atom.

The compound is named as a *C*-substituted monosaccharide. The group having priority according to the Sequence Rule ([13], Section E) is regarded as equivalent to OH for assignment of configuration. Any potential ambiguity (particularly when substitution is at the carbon atom where ring formation occurs) should be avoided by use of the *R,S* system to specify the modified stereocentre.

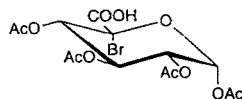
Examples:



2-*C*-Phenyl- α -D-glucopyranose



2-*C*-Acetamido-2,3,4,6-tetra-*O*-acetyl- α -D-mannopyranosyl fluoride

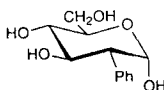


(5*R*)-1,2,3,4-Tetra-*O*-acetyl-5-bromo- α -D-*xylo*-hexopyranuronic acid
or 1,2,3,4-tetra-*O*-acetyl-5-bromo- β -L-idopyranuronic acid

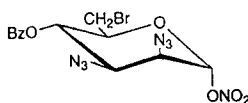
2-Carb-16.2. Replacement of OH at a non-terminal, non-anomeric carbon atom

The compound is named as a substituted derivative of a deoxy sugar. The group replacing OH determines the configurational description. Any potential ambiguity should be dealt with by the alternative use of the *R,S* system to specify the modified stereocentre.

Examples:



2-Deoxy-2-phenyl- α -D-glucopyranose or 2-deoxy-2-*C*-phenyl- α -D-glucopyranose
or (2*F*)-2-deoxy-2-phenyl- α -D-*arabino*-hexopyranose



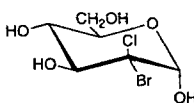
2,3-Diazo-4-*O*-benzoyl-6-bromo-2,3,6-trideoxy- α -D-mannopyranosyl nitrate

Note. Use of the symbol *C*- is essential only in cases of potential ambiguity, to make clear that substitution is at carbon rather than at a heteroatom (cf. 2-Carb-18.2); however, it may also be used for emphasis.

2-Carb-16.3. Unequal substitution at a non-terminal carbon atom

The compound is named as a disubstituted deoxy sugar. Configuration is determined by regarding the substituent having priority according to the Sequence Rule ([13], Section E), as equivalent to OH. Any potential ambiguity should be dealt with by the alternative use of the *R,S* system to specify the modified stereocentre.

Example:

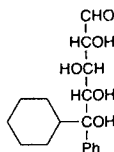


(2*F*)-2-Bromo-2-chloro-2-deoxy- α -D-*arabino*-hexose
or 2-bromo-2-chloro-2-deoxy- α -D-glucopyranose
(Br has priority over Cl)

2-Carb-16.4. Terminal substitution

If substitution at the terminal carbon atom of the carbohydrate chain creates a chiral centre, the stereochemistry is indicated by the *R,S* system.

Example:

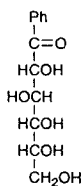


(5*F*)-5-*C*-Cyclohexyl-5-*C*-phenyl-D-xylose

Note. A monosaccharide with a terminal methyl group is named as a deoxy sugar, not as a *C*-methyl derivative.

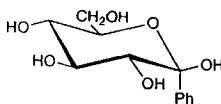
Substitution of aldehydic H by a ring or ring system is indicated simply with a *C*-substituent prefix.

Examples:



1-C-Phenyl-D-glucose

not 1-C-phenyl-D-gluc-hex-1-ulose

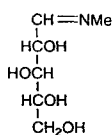


1-C-Phenyl- β -D-glucopyranose

2-Carb-16.5. Replacement of carbonyl oxygen by nitrogen (imines, oximes, hydrazones, osazones etc.)

The imino analogue of a monosaccharide may be named as an imino-substituted deoxy alditol.

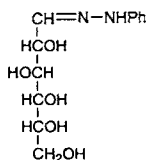
Example:



1-Deoxy-1-(methylimino)-D-xylitol

Oximes, hydrazones and analogues are named directly as oxime or hydrazone derivatives etc.

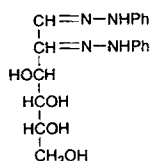
Example:



D-Glucose phenylhydrazone

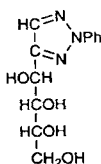
The vicinal dihydrazones formed from monosaccharides with arylhydrazines have been called arylosazones, but are preferably named as ketoaldose bis(phenylhydrazones)

Example:



D-*arabino*-Hexos-2-ulose bis(phenylhydrazone)
or D-*arabino*-hex-2-ulose phenylosazone

The triazoles formed on oxidising arylosazones (commonly called osotriazoles) may also be named as triazolalditols.



D-*arabino*-Hexos-2-ulose phenylosotriazole
or (1*R*)-1-(2-phenyl-2*H*-1,2,3-triazol-4-yl)-D-erythritol
or 2-phenyl-4-(D-*arabino*-1,2,3,4-tetrahydroxybutyl)-2*H*-1,2,3-triazole

2-Carb-16.6. Isotopic substitution and isotopic labelling

Rules for designating isotopic substitution and labelling are given in [13] (Section H). Parentheses indicate substitution; square brackets indicate labelling. The locant U indicates uniform labelling.

Examples:

D-(1-¹³C)Glucose (substitution)

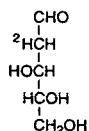
D-(2-²H)Mannose (substitution)

L-[U-¹⁴C]Arabinose (labelling)

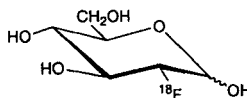
D-[1-³H]Galactose (labelling)

When isotopic substitution creates a centre of chirality, configuration is defined as for other types of substitution (see 2-Carb-16.1 to 2-Carb-16.4).

Example:



2-Deoxy-D-(2-²H)lyxose (substituted)
or (2*S*)-2-deoxy-D-*threo*-(2-²H)pentose



2-Deoxy-2-[¹⁸F]fluoro-D-glucose (labelled)
or (2*R*)-2-deoxy-2-[¹⁸F]fluoro-D-*arabino*-hexose

2-Carb-17. Unsaturated monosaccharides*

2-Carb-17.1. General principles

This section relates to the introduction of a double or triple bond between two contiguous carbon atoms of the backbone chain of a monosaccharide derivative. A double bond between a carbon atom of the backbone chain and an atom outside that chain, or a double or triple bond between two carbon atoms outside the backbone chain, will be treated according to the normal rules of organic nomenclature [13,14].

2-Carb-17.2. Double bonds

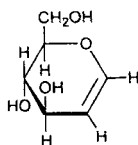
Monosaccharide derivatives having a double bond between two contiguous carbon atoms of the backbone chain are named by inserting, into the name for the corresponding fully saturated derivative, the infix 'x-en'. The infix is placed directly after the stem name that designates the chain length of the sugar. The locant *x* is the lower-numbered carbon atom involved in the double bond. Steric relations at a double bond are designated, if necessary, by the standard stereosymbols '(Z)-' and '(E)-' preceding the whole name ([13], Section E). For multiple double bonds, infixes such as 'x,y-dien' are used (preceded by an inserted 'a' for euphony).

Note 1. The term 'glycal' is a non-preferred, trivial name for cyclic enol ether derivatives of sugars having a double bond between carbon atoms 1 and 2 of the ring. It should not be used or modified as a class name for monosaccharide derivatives having a double bond in any other position.

Note 2. Following the principle of first naming the saturated derivative, compounds having a C=CR-O- group as part of a ring system are named as unsaturated derivatives of anhydro alditols if R is hydrogen or carbon; if R is a halogen, chalcogen, or nitrogen-family element, the resulting name is that of a glycenose or glycenosyl derivative.

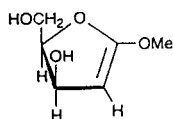
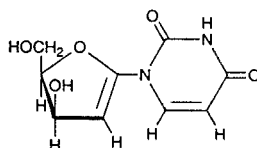
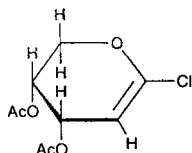
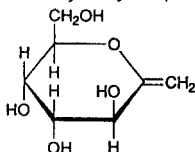
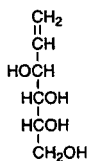
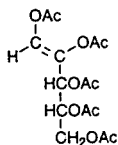
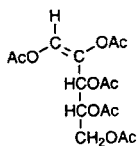
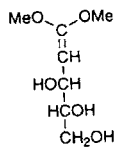
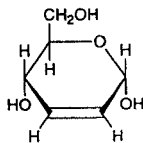
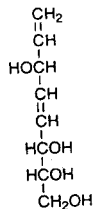
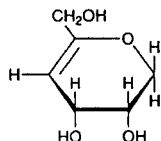
Note 3. The symbols (Z)- and (E)- may be omitted when the double bond is located within a ring system of six atoms or less, as steric constraints in such systems normally permit only one form.

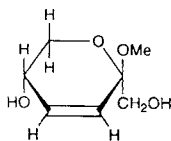
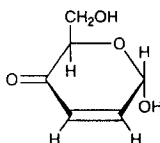
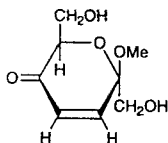
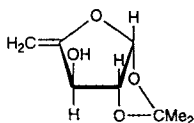
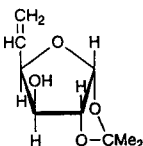
Examples:



1,5-Anhydro-2-deoxy-D-*arabino*-hex-1-enitol (non-preferred trivial name D-glucal)

* This is based on the 1980 recommendations [5]. Some examples have been omitted.

Methyl 2-deoxy-D-*threo*-pent-1-enofuranoside1-(2-Deoxy-D-*threo*-pent-1-enofuranosyl)uracil3,4-Di-*O*-acetyl-2-deoxy-D-*erythro*-pent-1-enopyranosyl chloride2,6-Anhydro-1-deoxy-D-*altra*-hept-1-enitol
(alphabetic preference over 2,6-anhydro-7-deoxy-D-*tal*o-hept-6-enitol)1,2-Dideoxy-D-*arabino*-hex-1-enitol(Z)-1,2,3,4,5-Penta-*O*-acetyl-D-*erythro*-pent-1-enitol(E)-1,2,3,4,5-Penta-*O*-acetyl-D-*erythro*-pent-1-enitol2-Deoxy-D-*threo*-pent-1-enose dimethyl acetal2,3-Dideoxy- α -D-*erythro*-hex-2-enopyranose1,2,4,5-Tetradeoxy-D-*arabino*-octa-1,4-dienitol1,5-Anhydro-4-deoxy-D-*erythro*-hex-4-enitol
(enantiomeric precedence over 2,6-anhydro-3-deoxy-L-*erythro*-hex-2-enitol)

Methyl 3,4-dideoxy- β -D-glycero-hex-3-en-2-ulopyranoside2,3-Dideoxy- α -D-glycero-hex-2-enopyranos-4-uloseMethyl 3,4-dideoxy- β -D-glycero-hept-3-en-2-ulopyranosid-5-ulose5-Deoxy-1,2-O-isopropylidene- β -L-threo-pent-4-enofuranose5,6-Dideoxy-1,2-O-isopropylidene- α -D-xylo-hex-5-enofuranose

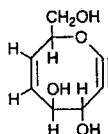
2-Carb-17.3. Triple bonds and cumulative double bonds

Monosaccharide derivatives having a triple bond or cumulative double bonds in the backbone chain are named by the methods of 2-Carb-17.2, with the infix '*n-yn*' for a triple bond and infixes such as '*i,j-dien*' for cumulative double bonds.

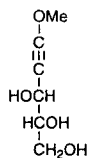
Note. This approach was not included in [5].

Alternatively they can be named on the basis of the corresponding fully saturated sugar by using the appropriate number of dehydro and deoxy prefixes (deoxy operations are regarded as formally preceding dehydro operations). The prefixes are placed in alphabetical order before the stem name.

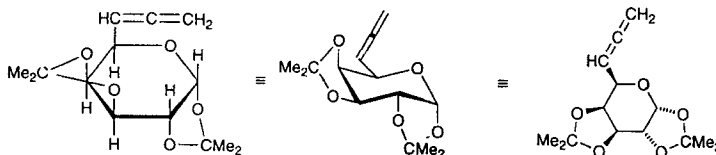
Examples:



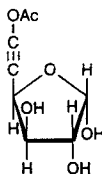
(*Z*)-1,7-Anhydro-2,5,6-trideoxy-D-xylo-oct-5-en-1-ynitol
or (*Z*)-1,7-anhydro-1,1,2,2-tetrahydro-2,5,6-trideoxy-D-xylo-oct-5-enitol



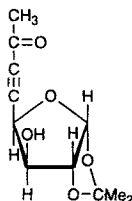
2-Deoxy-1-*O*-methyl-D-*threo*-pent-1-ynitol
or 1,1,2,2-tetrahydro-2-deoxy-1-*O*-methyl-D-*threo*-pentitol



6,7,8-Trideoxy-1,2:3,4-di-*O*-isopropylidene- α -D-*galacto*-octa-6,7-dienopyranose
or 6,7,8-tetrahydro-6,7,8-trideoxy-1,2:3,4-di-*O*-isopropylidene- α -D-*galacto*-octopyranose



6-*O*-Acetyl-5-deoxy- α -D-*xylo*-hex-5-ynofuranose
or 6-*O*-acetyl-5,5,6,6-tetrahydro-5-deoxy- α -D-*xylo*-hexofuranose



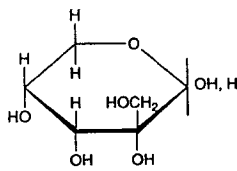
5,6,8-Trideoxy-1,2-*O*-isopropylidene- α -D-*xylo*-oct-5-ynofuranos-7-ulose
or 5,5,6,6-tetrahydro-5,6,8-trideoxy-1,2-*O*-isopropylidene- α -D-*xylo*-octofuranos-7-ulose

2-Carb-18. Branched-chain sugars*

2-Carb-18.1. Trivial names

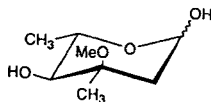
Several branched monosaccharides have trivial names, some established by long usage. Examples are given below, together with systematic names for the (cyclic or acyclic) forms illustrated. (See also the alphabetical listing of trivial names in the Appendix.) Enantiomers of the sugars listed should be named systematically.

Examples:

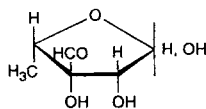


Hamamelose
2-*C*-(Hydroxymethyl)-D-ribofuranose

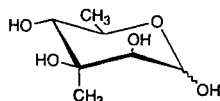
* This is a modified form of the 1980 recommendations [4]. Priority is now given to naming cyclic forms, since in most cases branched-chain monosaccharides will form cyclic hemiacetals or hemiketals.



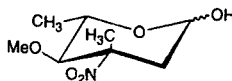
Cladinose
2,6-Dideoxy-3-C-methyl-3-O-methyl-L-ribo-hexopyranose



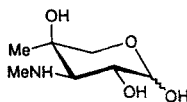
Streptose
5-Deoxy-3-C-formyl-L-lyxofuranose



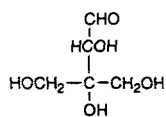
6-Deoxy-3-C-methyl-D-mannopyranose
(Evalose)



2,3,6-Trideoxy-3-C-methyl-4-C-methyl-3-nitro-L-arabino-hexopyranose
(Evernitrose)

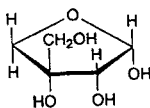


3-Deoxy-4-C-methyl-3-methylamino-L-arabinopyranose
(Garosamine)



D-Apiose (Api)
3-C-(Hydroxymethyl)-D-glycero-tetrose

Note. For the cyclic forms of apiose, systematic names are preferred, e.g.



3-C-(Hydroxymethyl)- α -D-erythro-furanose

[The name α -D-*erythro*-apiofuranose is ambiguous; Chemical Abstracts Service (CAS) uses the trivial name D-apio- α -D-furanose; Beilstein gives (3*R*)- α -D-apiofuranose]

2-Carb-18.2. Systematic names

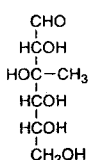
A branched-chain monosaccharide is named as a substituted parent unbranched monosaccharide, as outlined in 2-Carb-16.1 to 2-Carb-16.4.

Note. *C*-Locants are essential only where there is potential ambiguity, to make clear whether substitution is at carbon or at a heteroatom (cf. 2-Carb-16); however, they may also be used for emphasis.

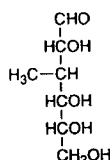
2-Carb-18.3. Choice of parent

If the branched monosaccharide forms a cyclic hemiacetal or hemiketal, the chain which includes the ring atoms rather than any alternative open chain must be the basis of the name. Otherwise the parent is chosen according to the principles given in 2-Carb-2.1.

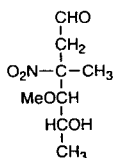
Examples (see also Chart V):



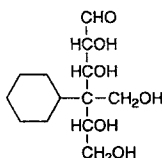
3-C-Methyl-D-glucose
(configuration determined by OH)



3-Deoxy-3-methyl-D-glucose
(configuration determined by CH₃)



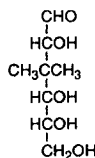
2,3,6-Trideoxy-3-C-methyl-4-O-methyl-3-nitro-D-lyxo-hexopyranose
(nitrogen has priority over carbon for determining configuration)



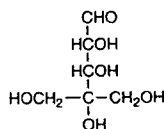
4-Cyclohexyl-4-deoxy-4-(hydroxymethyl)-D-allose
[oxygen (in CH₂OH) has priority over carbon (in cyclohexyl) at C-4]
or (4*R*)-4-cyclohexyl-4-deoxy-4-(hydroxymethyl)-D-*ribo*-hexose

If the two substituents at the branch point are identical, so that this centre has become achiral, the stereochemistry is specified as described in 2-Carb-8.4.

Examples:

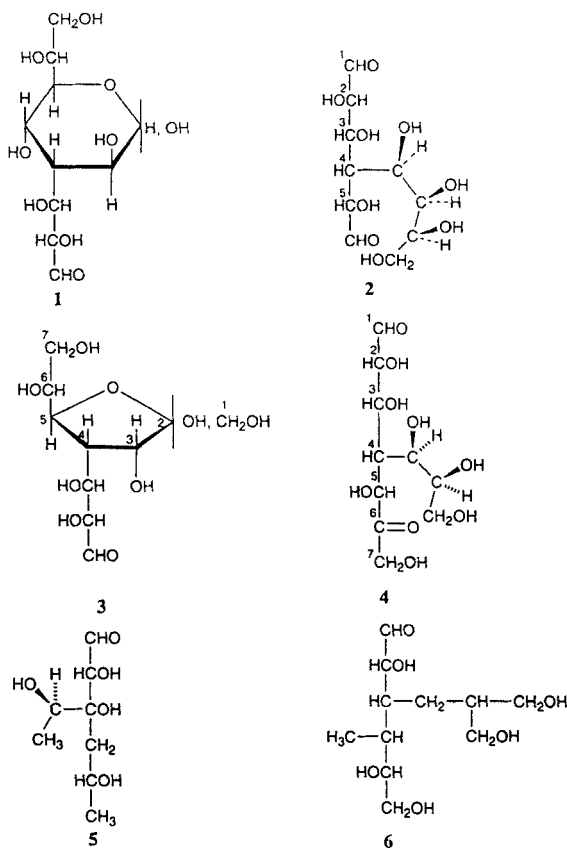


3-Deoxy-3,3-dimethyl-D-ribo-hexose



4-C-(Hydroxymethyl)-D-erythro-pentose

Note. Cyclization of the second example between C-1 and a CH₂OH group would necessitate a three-centre configurational prefix for the ring form.



- 1** 3-Deoxy-3-[(1*R*,2*S*)-1,2-dihydroxy-3-oxopropyl]-*D*-glycero-*D*-*altro*-heptopyranose
 or 3-deoxy-3-(*D*-*threo*-1,2-dihydroxy-3-oxopropyl)-*D*-glycero-*D*-*altro*-heptopyranose
 (not the alternative open-chain six-carbon dialdose or eight-carbon aldose, cf. **2**)
- 2** 4-Deoxy-4-(*L*-*ribo*-1,2,3,4-tetrahydroxybutyl)-*D*-*altro*-hexodialdose
- 3** 4-Deoxy-4-[(1*R*,2*R*)-1,2-dihydroxy-3-oxopropyl]-*D*-*allo*-heptulo-2,5-furanose
 or 4-deoxy-4-(*D*-*erythro*-1,2-dihydroxy-3-oxopropyl)-*D*-*allo*-heptulo-2,5-furanose
 (not the alternative ketoaldose, cf. **4**)
- 4** 4-Deoxy-4-[(1*R*,2*S*)-1,2,3-trihydroxypropyl]-*L*-*tal*o-heptos-6-ulose
 or 4-deoxy-4-(*L*-*erythro*-1,2,3-trihydroxypropyl)-*L*-*tal*o-heptos-6-ulose
- 5** 4,6-Dideoxy-3-*C*-(*D*-*glycero*-1-hydroxyethyl)-*D*-*ribo*-hexose
 (not the alternative pentose)
- 6** 3,4-Dideoxy-3-[3-hydroxy-2-(hydroxymethyl)propyl]-4-*C*-methyl-*L*-mannose
 (not the alternative *threo*-hexose)

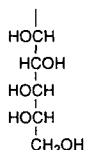
Chart V. Choice of parent in branched-chain monosaccharides. In the first names given for examples **1**, **3** and **4**, side-chain configuration is specified by use of *R* and *S*. This approach is generally preferred in all but the simplest cases, as less open to misinterpretation.

Note. These recommendations may give rise to very different names for cyclic and acyclic forms of the same basic structures, resulting from different priorities. Thus, in Chart V, structures **1** and **2** are virtually identical, differing only by cyclization. The same holds for structures **3** and **4**.

2-Carb-18.4. Naming the branches

Each branch will be named as an alkyl or substituted alkyl group replacing a hydrogen atom at the branch point of the parent chain. Within the branches, configurations around asymmetric centres can either be indicated using the *R,S*-system or, if they are carbohydrate-like and assignment is straightforward, by the use of the configurational prefix. For this purpose, and in the absence of a carbonyl group (or a terminal COOH or its equivalent) in the branch, the point of attachment of the branch (on the main chain) is regarded as equivalent to an aldehyde group.

Example:



L-*gluco*-1,2,3,4,5-Pentahydroxypentyl

If there is a carbonyl group in the branch (or a terminal COOH or its equivalent), its position (assigned lowest number when stereochemistry is being considered) is used to define the configurational prefix (see examples 1 and 3 in Chart V). Use of the *R,S* system is generally preferred, as less open to misinterpretation.

For an alternative approach to naming carbohydrate residues as substituents see 2-Carb-31.2 [which would give the name (1*R*)- or (1*S*)-L-arabinitol-1-C-yl for the above example, depending on the ligands at the branch point].

2-Carb-18.5. Numbering

The carbon atoms of the parent chain are numbered according to 2-Carb-2.2.1. If a unique numbering is required for the branch(es) (e.g. for X-ray or NMR work), the carbon atoms may be given the locant of the appropriate branch point, with the internal branch locant as superscript, e.g. 4² for position 2 of the branch at position 4 of the main chain. This style of branch numbering is not to be used for naming purposes: e.g. the side-chain-methylated derivative of compound 5 is named 4,6-dideoxy-3-*C*-[(*R*)-1-methoxyethyl]-D-*ribo*-hexose, and not as a 3¹-*O*-methyl derivative.

2-Carb-18.6. Terminal substitution

See 2-Carb-16.4.

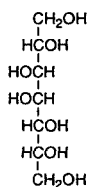
2-Carb-19. Alditols

2-Carb-19.1. Naming

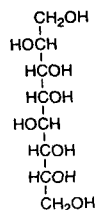
Alditols are named by changing the suffix '-ose' in the name of the corresponding aldose into '-itol'.

If the same alditol can be derived from either of two different aldoses, or from an aldose or a ketose, preference is ruled by 2-Carb-2.1 or 2.2.2 as appropriate.

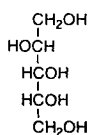
Examples:



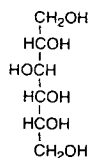
D-*glycero*-D-*galacto*-Heptitol
not L-*glycero*-D-*manno*-heptitol



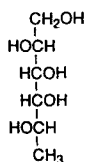
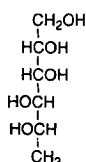
D-*erythro*-L-*galacto*-Octitol
not D-*threo*-L-*gulo*-octitol



D-Arabinitol (Ara-ol) not D-lyxitol

D-Glucitol (Glc-ol) not L-gulitol
(the trivial name sorbitol is not recommended)

The trivial names fucitol and rhamnitol are allowed for the alditols corresponding to the 6-deoxy sugars fucose and rhamnose.

L-Fucitol (L-Fuc-ol) or 1-deoxy-D-galactitol
not 6-deoxy-L-galactitol (cf. 2-Carb-2.2.3.1)

L-Rhamnitol (L-Rha-ol) or 1-deoxy-L-mannitol

2-Carb-19.2. *meso* Forms

Alditols that are symmetric and therefore optically inactive - the *meso* forms - can be designated by the prefix *meso*-.

Examples:

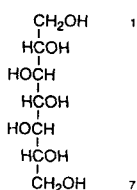
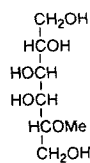
meso-Erythritol

meso-Ribitol

meso-Galactitol

The prefix D or L must be given when a derivative of a *meso* form has become asymmetric by substitution. It is also necessary to define the configurational prefixes as D or L in the case where there are more than four contiguous asymmetric carbon atoms.

Examples:

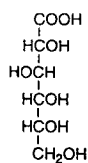
*meso*-D-glycero-L-ido-Heptitol
not L-glycero-D-ido-heptitol; cf. 2-Carb-2.2.35-O-Methyl-D-galactitol
not 2-O-methyl-L-galactitol

2-Carb-20. Aldonic acids

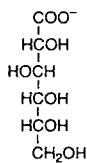
2-Carb-20.1. Naming

Aldonic acids are divided into aldotronic acid, aldotetronic acids, aldopentonic acids, aldohexonic acids, etc., according to the number of carbon atoms in the chain. The names of individual compounds of this type are formed by replacing the ending '-ose' of the systematic or trivial name of the aldose by '-onic acid'.

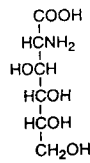
Examples:



D-Gluconic acid



D-Gluconate



2-Amino-2-deoxy-D-gluconic acid

2-Carb-20.2. Derivatives

Salts are named by changing the ending ‘-onic acid’ to ‘-onate’, denoting the anion. If the counter ion is known, it is given before the aldionate name.

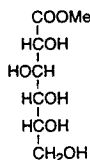
Example:

Sodium D-gluconate

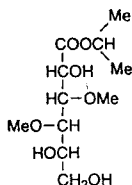
Esters derived from the acid function are also named using the ending ‘-onate’. The name of the alkyl (aryl, etc.) group is given before the aldionate name. Alternative periphrase names like ‘aldonic acid alkyl (aryl, etc.) ester’ may be suitable for an index.

Amides are designated by the ending ‘-onamide’, and nitriles by the ending ‘-ononitrile’.

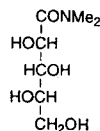
Examples:



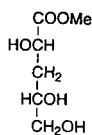
Methyl D-gluconate



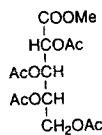
Isopropyl 3,4-di-O-methyl-L-mannonate



N,N-Dimethyl-L-xylonamide



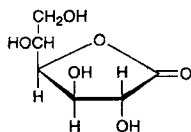
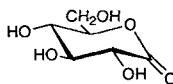
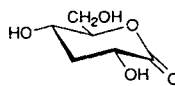
Methyl 3-deoxy-D-threo-pentionate



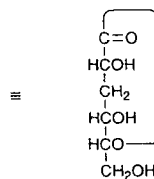
Methyl tetra-O-acetyl-L-arabinonate

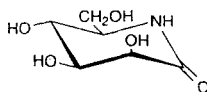
Lactones are named with the ending ‘-onolactone’. The locants must be given (in the form ‘-ono-*i,j*-lactone’); that of the carbonyl group (*i*) is cited first, and that of the oxygen (*j*) second (see examples below). Periphrase names (see alternatives in parentheses) appear widely in the literature but are not recommended. *Lactams* are named similarly by use of the ending ‘-onolactam’.

Examples:

D-Glucono-1,4-lactone
(D-Gluconic acid γ -lactone)D-Glucono-1,5-lactone
(D-Gluconic acid δ -lactone)

3-Deoxy-D-ribo-hexono-1,5-lactone

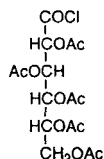




5-Amino-5-deoxy-D-mannono-1,5-lactam

Acyl halides are named by changing the ending '-onic acid' to '-onyl halide'.

Example:



Penta-O-acetyl-D-gluconoyl chloride

More complicated examples of general principles for naming acid derivatives can be found elsewhere [13,14].

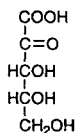
2-Carb-21. Ketoaldonic acids

2-Carb-21.1. Naming

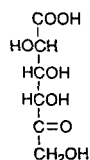
Names of individual ketoaldonic acids are formed by replacing the ending '-ulose' of the corresponding ketose by '-ulosonic acid', preceded by the locant of the ketonic carbonyl group. The anion takes the ending '-ulosonate'. The numbering starts at the carboxy group.

In glycosides derived from ketoaldonic acids, the ending is '-ulosidonic acid', with appropriate ring-size infix, e.g. '-ulopyranosidonic acid'.

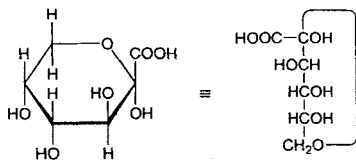
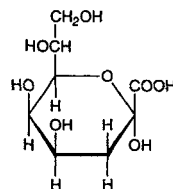
Examples:



D-erythro-Pent-2-ulosonic acid



D-arabino-Hex-5-ulosonic acid

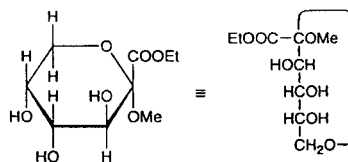
 α -D-arabino-Hex-2-ulopyranosonic acid3-Deoxy- α -D-manno-oct-2-ulopyranosonic acid

Note. The last of the above examples is one of the possible forms of the compound referred to by the three-letter symbol Kdo (formerly the abbreviation KDO, from the previously allowed trivial name ketodeoxyoctonic acid). Similarly the symbol Kdn for the C_9 sugar 3-deoxy-D-glycero-D-galacto-non-2-ulopyranosonic acid is widely used.

2-Carb-21.2. Derivatives

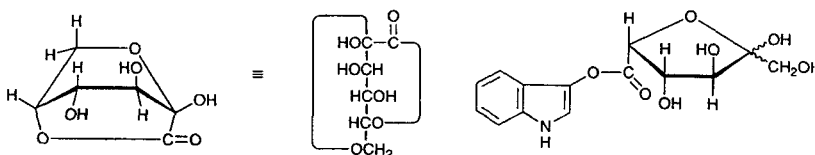
Esters, lactones, lactams, acyl halides etc. are named by modifying the ending '-ic acid' as described for aldonic acids (2-Carb-20.2).

Examples:



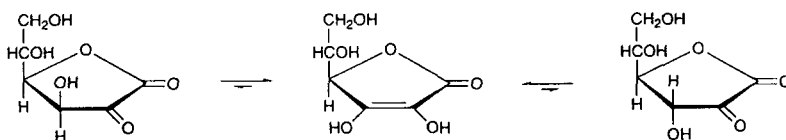
Ethyl (methyl α -D-arabino-hex-2-ulopyranosid)onate

Note. The parentheses are inserted to distinguish between the ester alkyl group (cited first) and the glycosidic *O*-alkyl group.



β -D-arabino-Hex-2-ulopyranosono-1,5-lactone

Indol-3-yl D-xylo-hex-5-ulofuranosonate;
trivial name isatan B



L-xylo-Hex-2-ulosono-1,4-lactone

L-threo-Hex-2-enono-1,4-lactone

L-lyxo-Hex-2-ulosono-1,4-lactone

(L-Ascorbic acid is the equilibrium mixture of all three isomers)

2-Carb-22. Uronic acids

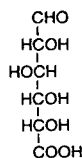
2-Carb-22.1. Naming and numbering

The names of the individual compounds of this type are formed by replacing (a) the '-ose' of the systematic or trivial name of the aldose by '-uronic acid', (b) the '-oside' of the name of the glycoside by '-osiduronic acid' or (c) the '-osyl' of the name of the glycosyl group by '-osyluronic acid'. The carbon atom of the (potential) aldehydic carbonyl group (*not* that of the carboxy group as in normal systematic nomenclature [13,14]) is numbered 1 (see 2-Carb-2.1, note 1).

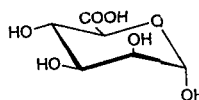
2-Carb-22.2. Derivatives

Derivatives of these acids formed by change in the carboxy group (salts, esters, lactones, acyl halides, amides, nitriles, etc.) are named according to 2-Carb-20.2. The anion takes the ending '-uronate'. Esters are also named using the ending '-uronate'.

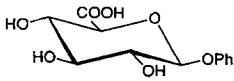
Examples:



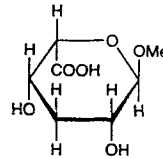
D-Glucuronic acid



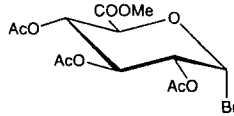
α -D-Mannopyranuronic acid



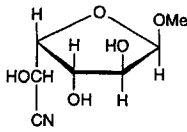
Phenyl β -D-glucopyranosiduronic acid
not phenyl β -D-glucuronoside or phenyl glucuronide



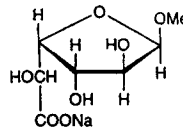
Methyl α -L-idopyranosiduronic acid



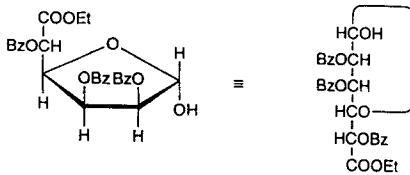
Methyl 2,3,4-tri-O-acetyl- α -D-glucopyranosyluronate bromide



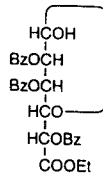
Methyl α -L-glucofuranosiduronitrile



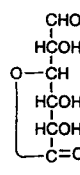
Sodium (methyl α -L-glucofuranosid)uronate



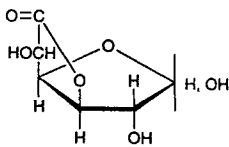
Ethyl 2,3,5-tri-O-benzoyl- α -D-mannofuranuronate



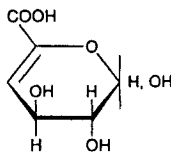
D-Glucurono-6,3-lactone



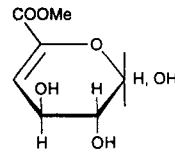
Methyl α -D-glucofuranosidurono-6,3-lactone



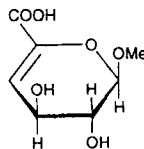
D-Glucufuranurono-6,3-lactone



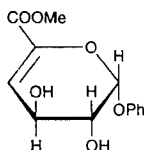
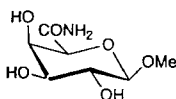
4-Deoxy-L-*threo*-hex-4-enopyranuronic acid



Methyl 4-deoxy-L-*threo*-hex-4-enopyranuronate



Methyl 4-deoxy- α -L-*threo*-hex-4-enopyranosiduronic acid

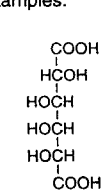
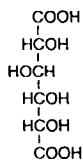
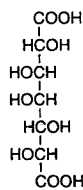
Methyl (phenyl 4-deoxy- β -L-threo-hex-4-enopyranosid)uronateMethyl β -D-galactopyranosiduronamide

2-Carb-23. Aldaric acids

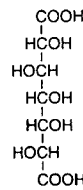
2-Carb-23.1. Naming

Names of individual aldaric acids are formed by replacing the ending '-ose' of the systematic or trivial name of the parent aldose by '-aric acid'. Choice between possible names is based on 2-Carb-2.2.2.

Examples:

L-Altriaric acid
not L-talaric acidD-Glucaric acid
not L-gularic acidL-glycero-D-galacto-Heptaric acid
not L-glycero-D-gluco-heptaric acid

≡

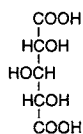
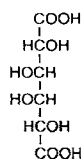
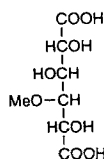


2-Carb-23.2. meso Forms

To the names of aldaric acids that are symmetrical, which therefore have no D- or L- prefix, the prefix '*meso*' may be added for the sake of clarity. Examples: *meso*-erythraric acid, *meso*-ribaric acid, *meso*-xylic acid, *meso*-allaric acid, *meso*-galactaric acid.

The D or L prefix must however be used when a *meso*-aldaric acid has become asymmetric as a result of substitution.

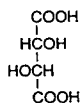
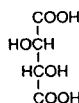
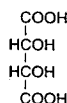
Examples:

*meso*-Xylic acid*meso*-Galactaric acid4-O-Methyl-D-galactaric acid
not 3-O-methyl-L-galactaric acid

2-Carb-23.3. Trivial names

For the tetraric acids, the trivial name tartaric acid remains in use, with the stereochemistry given using the *R,S* system. Esters are referred to as 'tartrates' (the second 'a' is elided).

Examples:

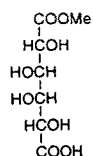
(2*R*,3*R*)- or (+)-Tartaric acid
or L-threaric acid(2*S*,3*S*)- or (-)-Tartaric acid
or D-threaric acid(2*R*,3*S*)- or *meso*-Tartaric acid
or erythraric acid

Note. In the older literature, there is confusion about the use of D and L in the case of tartaric acids. It is therefore recommended to use the *R,S* system in this case.

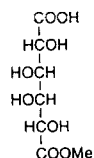
2-Carb-23.4. Derivatives

Derivatives formed by modifying the carboxy group (salts, esters, lactones, lactams, acyl halides, amides, nitriles etc.) are named by the methods of 2-Carb-20.2. Dilactones, half-esters, amic acids etc. are named by the methods of [13, 14]. In cases of ambiguity, locants should be specified.

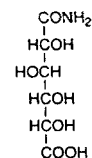
Examples:



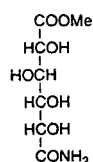
1-Methyl hydrogen D-galactarate



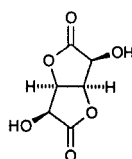
6-Methyl hydrogen D-galactarate



D-Glucar-1-amic acid



Methyl D-glucar-6-amate



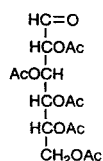
D-Mannaro-1,4:6,3-dilactone

2-Carb-24. O-Substitution

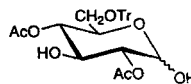
2-Carb-24.1. Acyl (alkyl) names

Substituents replacing the hydrogen atom of an alcoholic hydroxy group of a saccharide or saccharide derivative are denoted as *O*-substituents. The '*O*-' locant is not repeated for multiple replacements by the same atom or group. Number locants are used as necessary to specify the positions of substituents; they are not required for compounds fully substituted by identical groups. Alternative periphrase names for esters, ethers, etc. may be useful for indexing purposes. For cyclic acetals see 2-Carb-28.

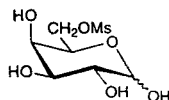
Examples:



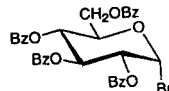
Penta-*O*-acetyl-*aldehydo*-D-glucose or *aldehydo*-D-glucose pentaacetate



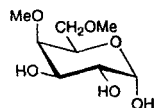
2,4-Di-*O*-acetyl-6-*O*-trityl-D-glucopyranose



6-*O*-Methanesulfonyl-D-galactopyranose or D-galactopyranose 6-methanesulfonate



Tetra-*O*-benzoyl- α -D-galactopyranosyl bromide



4,6-Di-*O*-methyl- α -D-galactopyranose

Note. Acyl substituents on anomeric OH are designated (as above) by *O*-acyl prefixes. However, anomeric *O*-alkyl derivatives are named as glycosides (see 2-Carb-33).

2-Carb-24.2. Phosphorus oxoacid esters

24.2.1. Phosphates

Of special biochemical importance are the esters of monosaccharides with phosphoric acid. They are generally termed phosphates (e.g. glucose 6-phosphate). In biochemical use, the term 'phosphate' indicates the phosphate residue regardless of the state of ionization or the counter ions.

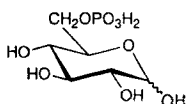
The prefix terms used for phosphate esters in organic nomenclature ([14], p.65) are '*O*-phosphono-' and '*O*-phosphonato-' for the groups (HO)₂P(O)- and (O⁻)₂P(O)- respectively, bonded to oxygen.

The term 'phospho-' is used for (HO)₂P(O)- or ionized forms in a biochemical context (see recommendations for the nomenclature of phosphorus-containing compounds [24]).

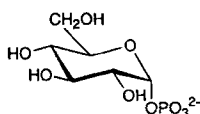
If a sugar is esterified with two or more phosphate groups, the compound is termed bisphosphate, triphosphate etc. (e.g. fructofuranose 1,6-bisphosphate). The term diphosphate denotes an ester with diphosphoric acid, e.g. adenosine 5'-diphosphate.

Note. In abbreviations, a capital P is used to indicate a terminal -PO₃H₂ group or a non-terminal -PO₂H- group (or dehydrated forms).

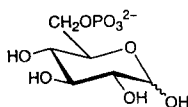
Examples:



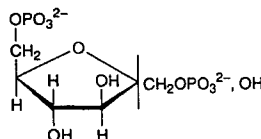
D-Glucopyranose 6-(dihydrogen phosphate)
or 6-*O*-phosphono-D-glucopyranose



α-D-Glucopyranosyl phosphate
(biochemical usage: glucose 1-phosphate) (Glc1P)



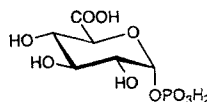
D-Glucopyranose 6-phosphate
(often shortened to glucose 6-phosphate)
or 6-*O*-phosphonato-D-glucopyranose
or 6-phospho-D-glucose (Glc6P)
(in a biochemical context)



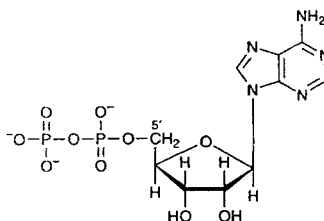
D-Fructofuranose 1,6-bisphosphate
(often shortened to fructose 1,6-bisphosphate)
or 1,6-di-*O*-phosphonato-D-fructofuranose
or 1,6-bisphospho-D-fructofuranose



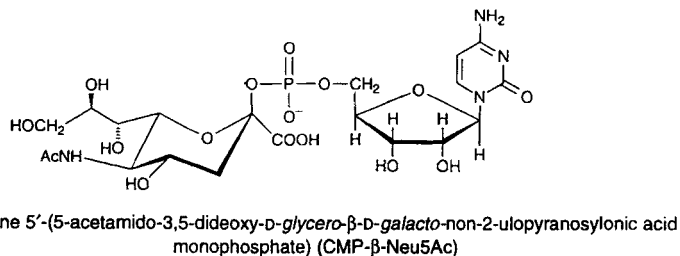
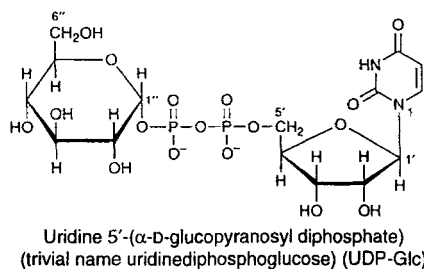
3-*O*-Phosphonato-D-glyceroyl phosphate
or 3-phospho-D-glyceroyl phosphate
or 1,3-bisphospho-D-glycerate (for biochemical usage)



α-D-Glucopyranuronic acid
1-(dihydrogen phosphate)
(biochemical usage: glucuronate 1-phosphate) (GlcA1P)



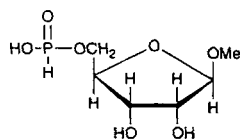
Adenosine 5'-diphosphate (ADP) or 5'-diphosphoadenosine



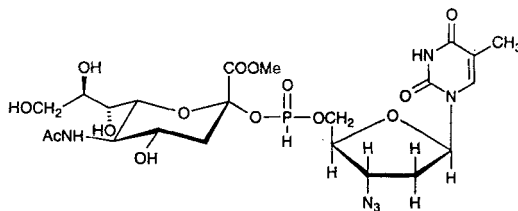
24.2.2. Phosphonates

The following examples illustrate the use of phosphonate terminology for esters of phosphonic acid, $\text{HP}(\text{O})(\text{OH})_2$. For formation of the alternative (substitutive) names, see 2-Carb-31.2.

Examples:



Methyl β -D-ribofuranoside 5-(hydrogen phosphonate)
or methyl 5-deoxy- β -D-ribofuranosid-5-yl hydrogen phosphonate

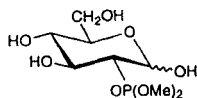


3'-Azido-3'-deoxythymidine 5'-[(methyl 5-acetamido-3,5-dideoxy-D-glycero- α -D-galacto-non-2-ulopyranosylonate) phosphonate]

Derivatives substituted on phosphorus are named by standard procedures [13, 14]; e.g. *P*-methyl derivatives are named as methylphosphonates.

Compounds with a phosphonate group linked by a P-C bond to a carbohydrate residue may be named as glycos-*n*-ylphosphonates (cf. 2-Carb-31.2) or as C-substituted carbohydrates (cf. amino sugars, 2-Carb-14).

Example:



2-Deoxy-2-dimethoxyphosphoryl-D-glucopyranose
(this usage of 'phosphoryl' is given in [13], Section D, Rule 5.68, and [14], p. 65)
or dimethyl 2-deoxy-D-glucopyranos-2-ylphosphonate

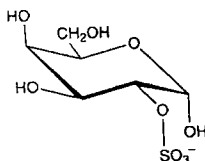
24.2.3. Phosphinates

Esters of phosphinic acid, $\text{H}_2\text{P}(\text{O})(\text{OH})$, are named by the same methods as used for phosphonates. For examples with two P–C bonds see 2-Carb-31.3.

2-Carb-24.3. Sulfates

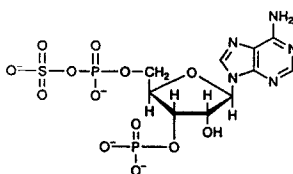
The prefix terms used for sulfuric esters are '*O*-sulfo-' and '*O*-sulfonato-', for the groups $(\text{HO})\text{S}(\text{O})_2^-$ and $(\text{O}^-)\text{S}(\text{O})_2^-$ respectively, bonded to oxygen. Sulfates may also be named by citing the word 'sulfate', preceded by the appropriate locant, after the carbohydrate name.

Example:



α -D-Galactopyranose 2-sulfate
or 2-*O*-sulfonato- α -D-galactopyranose

The mixed sulfuric phosphoric anhydride (PAdoPS or PAPS) of 3'-phospho-5'-adenylic acid is named as an acyl sulfate:



3'-Phospho-5'-adenylyl sulfate (PAPS)

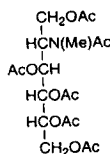
2-Carb-25. N-Substitution

Substitution, e.g. acylation, at the NH_2 group of an amino sugar can be dealt with in two different ways:

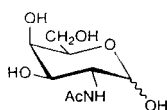
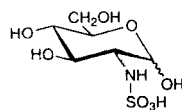
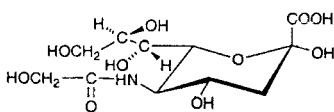
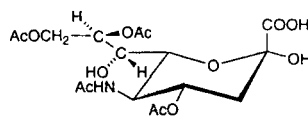
- The whole substituted amino group can be designated as a prefix, e.g. 2-acetamido- (or 2-butylamino-) 2-deoxy-D-glucose. For the purpose of the configurational prefix, the group is considered to take the place of the former OH group.
- If the amino sugar has a trivial name, the substitution is indicated by a prefix preceded by an italic capital *N*.

Note. In carbohydrate nomenclature, substitution at a heteroatom is normally indicated by citing the locant of the attached carbon atom, followed by a hyphen, and then the italicized heteroatom element symbol, e.g. 2-*O*-methyl, 5-*N*-acetyl. Substituents on the same kind of heteroatom are grouped (e.g. 2,3,4-tri-*O*-methyl), and substituents of the same kind are cited in alphabetical order of heteroatoms (e.g. 5-*N*-acetyl-4,8,9-tri-*O*-acetyl). The alternative format with superscript numerical locants (e.g. N^5, O^4, O^8, O^9 -tetraacetyl), used in some other areas of natural product chemistry, is unusual in carbohydrate names.

Examples:



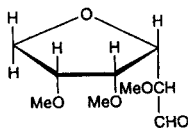
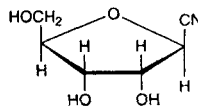
1,3,4,5,6-Penta-*O*-acetyl-2-deoxy-2-(*N*-methylacetamido)-D-glucitol

2-Acetamido-2-deoxy-D-galactopyranose
or *N*-acetyl-D-galactosamine2-Deoxy-2-sulfoamino-D-glucopyranose
or *N*-sulfo-D-glucosamine*N*-Glycolyl- α -neuraminic acid (α -Neu5Gc)
(D is implied in the trivial name)5-*N*-Acetyl-4,8,9-tri-*O*-acetyl- α -neuraminic acid
(α -Neu4,5,8,9Ac4)**2-Carb-26. Intramolecular anhydrides**

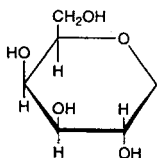
An intramolecular ether (commonly called an intramolecular anhydride), formally arising by elimination of water from two hydroxy groups of a single molecule of a monosaccharide (aldose or ketose) or monosaccharide derivative, is named by attaching the (detachable) prefix 'anhydro-' preceded by a pair of locants identifying the two hydroxy groups involved.

Note. Detachable prefixes are cited in alphabetical order along with any substituent prefixes.

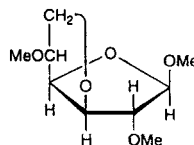
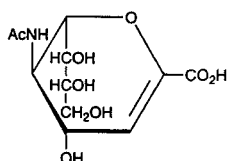
Examples:

3,6-Anhydro-2,4,5-tri-*O*-methyl-D-glucose

2,5-Anhydro-D-allononitrile



1,5-Anhydro-D-galactitol

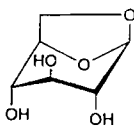
Methyl 3,6-anhydro-2,5-di-*O*-methyl- β -D-glucofuranoside

5-Acetamido-2,6-anhydro-3,5-dideoxy-D-glycero-D-galacto-non-2-enonic acid (Neu2en5Ac)

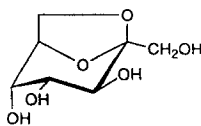
The compounds usually known as monosaccharide anhydrides or glycoside anhydrides (earlier 'glycosans'), formation of which involves the anomeric hydroxy group, are named by the same procedure. In these cases the order of preference of ring size designators is pyranose > furanose > septanose. However, three- or four-membered rings should normally be cited as 'anhydro' if there is a choice.

Trivial names for anhydro monosaccharides, though established by usage, are not recommended because of possible confusion with polysaccharide names based on the use of the termination '-an'.

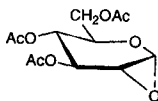
Examples:



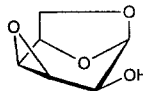
1,6-Anhydro- β -D-glucopyranose
not 1,5-anhydro- α -D-glucoseptanose
(older trivial name: levoglucosan)



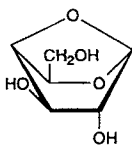
2,7-Anhydro- β -D-*altro*-hept-2-ulopyranose
(older trivial name: sedoheptulosan)



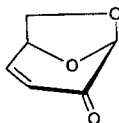
3,4,6-Tri-*O*-acetyl-1,2-anhydro- α -D-glucopyranose
not 3,4,6-tri-*O*-acetyl-1,5-anhydro- β -D-glucooxirose



1,6:3,4-Dianhydro- β -D-talopyranose



1,4-Anhydro- β -D-galactopyranose

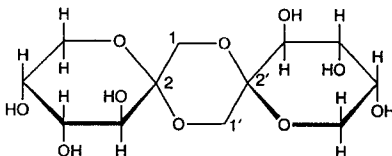


1,6-Anhydro-3,4-dideoxy- β -D-*glycero*-hex-3-enopyranos-2-ulose
(trivial name: levoglucosenone)

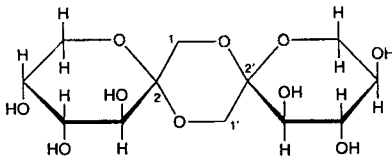
2-Carb-27. Intermolecular anhydrides

The cyclic product of condensation of two monosaccharide molecules with the elimination of two molecules of water (commonly called an intermolecular anhydride), is named by placing the word 'dianhydride' after the names of the two parent monosaccharides. When the two parent monosaccharides are different, the one preferred according to the order of preference given in 2-Carb-2.1 is cited first. The position of each anhydride link is indicated by a pair of locants showing the positions of the two hydroxy groups involved; the locants relating to one monosaccharide (in a mixed dianhydride, the second monosaccharide named) are primed. Both pairs of locants immediately precede the word 'dianhydride'.

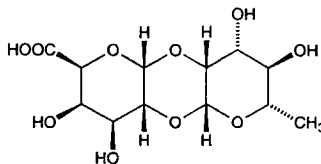
Examples:



α -D-Fructopyranose β -D-fructopyranose 1,2':1',2-dianhydride



α -D-Fructopyranose α -D-sorbopyranose 1,2':1',2-dianhydride

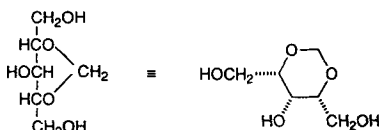


(α -D-Galactopyranuronic acid) β -L-rhamnopyranose 1,2':1',2-dianhydride

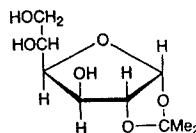
2-Carb-28. Cyclic acetals

Cyclic acetals formed by the reaction of saccharides or saccharide derivatives with aldehydes or ketones are named in accordance with 2-Carb-24.1, bivalent substituent names (formed by general organic nomenclature principles) being used as prefixes. In indicating more than one cyclic acetal grouping of the same kind, the appropriate pairs of locants are separated typographically when the exact placement of the acetal groups is known.

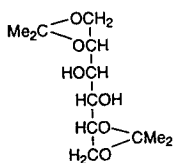
Examples:



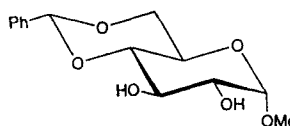
2,4-*O*-Methylenexylitol



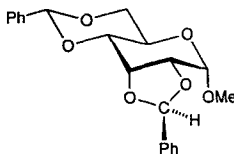
1,2-*O*-Isopropylidene- α -D-glucopyranose



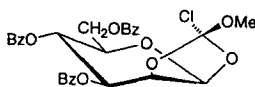
1,2:5,6-*O*-Di-*O*-isopropylidene-D-mannitol



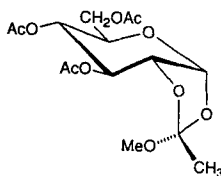
Methyl (*R*)-4-*O*-benzylidene- α -D-glucopyranoside



Methyl (*S*)-2,3:(*R*)-4,6-di-*O*-benzylidene- α -D-allopyranoside



3,4,6-Tri-*O*-benzoyl-[(*S*)-1,2-*O*-chloro(methoxy)methylene]- β -D-mannopyranose



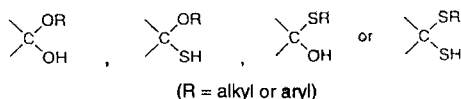
3,4,6-Tri-*O*-acetyl- α -D-glucopyranose (*R*)-1,2-(methyl orthoacetate)
or 3,4,6-tri-*O*-acetyl-[(*R*)-1,2-*O*-(1-methoxyethylidene)]- α -D-glucopyranose

Note 1. The last two examples contain cyclic ortho ester structures. These compounds are conveniently named as cyclic acetals.

Note 2. In the last four examples, new asymmetric centres have been introduced at the carbonyl carbon atom of the aldehyde or ketone that has reacted with the saccharide. When known, the stereochemistry at such a new centre is indicated by use of the appropriate *R* or *S* symbol ([13], Section E) placed in parentheses, immediately before the locants of the relevant prefix.

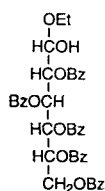
2-Carb-29. Hemiacetals, hemiketals and their thio analogues

The compounds obtained by transforming the carbonyl group of the acyclic form of a saccharide, or saccharide derivative, into the grouping:

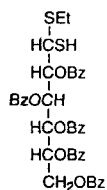


are named as indicated in 2-Carb-30, by using the terms 'hemiacetal', 'monothiohemiacetal', or 'dithiohemiacetal' (or the corresponding 'hemiketal' terms for ketone derivatives), as appropriate. The two isomers of a monothiohemiacetal are differentiated by use of *O* and *S* prefixes.

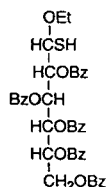
Examples:



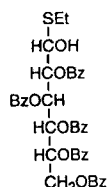
(1*S*)-2,3,4,5,6-Penta-*O*-benzoyl-D-glucose ethyl hemiacetal



(1*S*)-2,3,4,5,6-Penta-*O*-benzoyl-D-glucose ethyl dithiohemiacetal



(1*F*)-2,3,4,5,6-Penta-*O*-benzoyl-D-glucose *O*-ethyl monothiohemiacetal

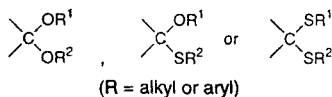


(1*S*)-2,3,4,5,6-Penta-*O*-benzoyl-D-glucose *S*-ethyl monothiohemiacetal

Note. In these compounds carbon atom number 1 has become chiral. When known, the stereochemistry at this new chiral centre is indicated using the *R,S* system ([13], Section E).

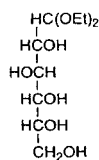
2-Carb-30. Acetals, ketals and their thio analogues

The compounds obtained by transforming the carbonyl group of a saccharide or saccharide derivative into the grouping:

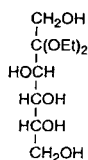


are named by placing after the name of the saccharide or saccharide derivative the term 'acetal', 'monothioacetal' or 'dithioacetal' (or the corresponding 'ketal' terms for ketone derivatives) as appropriate, preceded by the names of the groups R^1 and R^2 . With monothioacetals, the mode of bonding of two different groups R^1 and R^2 is indicated by the use of the prefixes *O* and *S*.

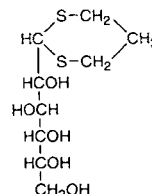
Examples:



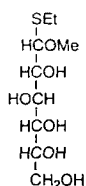
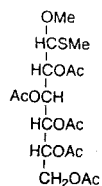
D-Glucose diethyl acetal



D-Fructose diethyl ketal



D-Glucose propane-1,3-diyl dithioacetal

(1*S*)-D-Glucose *S*-ethyl
O-methyl monothioacetal(1*R*)-2,3,4,5,6-Penta-O-acetyl-D-glucose
dimethyl monothioacetal

Note. In the last two examples, carbon atom 1 has become chiral. When known, the stereochemistry at this new chiral centre is indicated by the *R,S* system, as specified in 2-Carb-29.

2-Carb-31. Names for monosaccharide residues

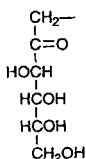
2-Carb-31.1. Glycosyl residues

The residue formed by detaching the anomeric hydroxy group from a monosaccharide is named by replacing the terminal 'e' of the monosaccharide name by '-yl'. The general name is 'glycosyl' residue. Terms of this type are widely used in naming glycosides and oligosaccharides. For examples (including glycosyl residues from uronic acids), see 2-Carb-33.2. The term 'glycosyl' is also used in radicofunctional names, e.g. for halides such as the glucopyranosyl bromide in 2-Carb-24.1 and the mannopyranosyl fluoride in 2-Carb-16.1, and esters such as the glucopyranosyl phosphate in 2-Carb-24.2.1 and the mannopyranosyl nitrate in 2-Carb-16.2.

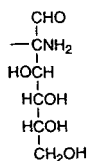
2-Carb-31.2 Monosaccharides as substituent groups

In order to produce names for structures in which it may be desirable for a non-carbohydrate portion to be cited as parent, prefix terms are required for carbohydrate residues linked through carbon or oxygen at any position on the main chain. These prefixes can be formed by replacing the final 'e' of the systematic or trivial name of a monosaccharide by '-*n*-C-yl', '-*n*-O-yl' or '-*n*-yl' (if there is no ambiguity). In each case the term '-yl' signifies loss of H from position *n*. At a secondary position (e.g. in 2-deoxy-D-glucos-2-yl, below) the free valency is regarded as equivalent to OH for assignment of configuration.

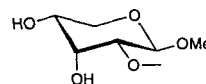
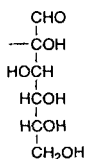
Examples:



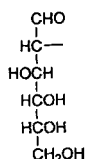
1-Deoxy-D-fructos-1-yl



2-Amino-2-deoxy-D-glucos-2-yl

(Methyl β -D-ribofuranosid-2-O-yl)

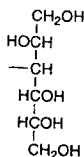
D-Glucos-2-C-yl



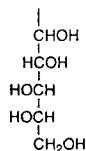
2-Deoxy-D-glucos-2-yl

The same endings can be used to form substituent prefixes for alditol residues.

Examples:



3-Deoxy-D-mannitol-3-yl

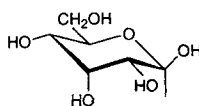


L-Arabinitol-1-C-yl (cf. 2-Carb-18.4)
(*R/S* to be specified at C-1)

The ending '-yl' without locants signifies loss of OH from the anomeric position (see 2-Carb-31.1). Loss of H from the anomeric OH is indicated by the ending '-yloxy', without locant. For examples see 2-Carb-33.

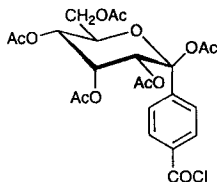
The situation in which the anomeric OH is retained but H is lost from the anomeric carbon atom is indicated by use of the ending '-yl' without locants in conjunction with the prefix '1-hydroxy-' (not by the ending '-1-C-yl'). **N.B.** In this case, the anomeric prefix α or β refers to the free valency, not the OH group.

Example:

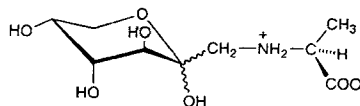


1-Hydroxy- α -D-allopyranosyl

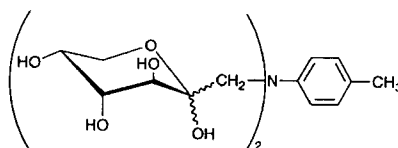
Examples of the use of substituent prefixes for carbohydrate residues:



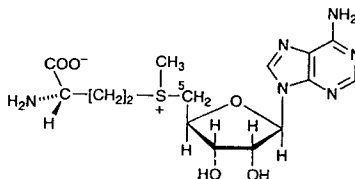
4-(1-Acetoxy-2,3,4,6-tetra-*O*-acetyl- α -D-allopyranosyl)benzoyl chloride



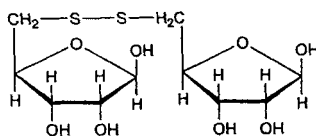
N-(1-Deoxy-D-fructopyranos-1-yl)-L-alanine



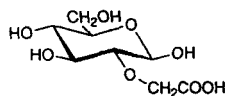
N,N-Bis-(1-deoxy-D-fructopyranos-1-yl)-*p*-toluidine



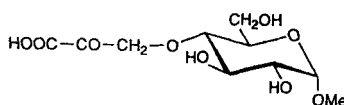
S-(5'-Deoxyadenosin-5'-yl)-L-methionine (AdoMet)
S-[(1-Adenin-9-yl)-1,5-dideoxy- β -D-ribofuranos-5-yl]-L-methionine
[trivial name *S*-adenosylmethionine (SAM)]



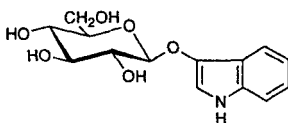
Bis(5-deoxy- β -D-ribofuranos-5-yl) disulfide
or bis(5-deoxy- β -D-ribofuranos-5-yl)disulfane



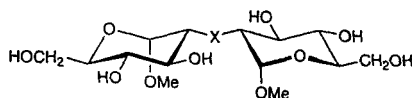
(β -D-Glucopyranos-2-O-yl)acetic acid
(more commonly named 2-O-carboxymethyl- β -D-glucopyranose; see 2-Carb-2.1, note 2)



(Methyl α -D-glucopyranosid-4-O-yl)pyruvic acid [or methyl 4-O-(oxalomethyl)- α -D-glucopyranoside]



3-(β -D-Glucopyranosyloxy)indole (or indol-3-yl β -D-glucopyranoside); trivial name indican



X = O

Methyl 2-O-(methyl 2-deoxy- α -D-glucopyranosid-2-yl)- α -D-glucopyranoside
or bis(methyl 2-deoxy- α -D-glucopyranosid-2-yl) ether

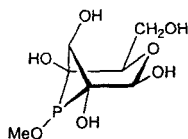
X = NH

Bis(methyl 2-deoxy- α -D-glucopyranosid-2-yl)amine

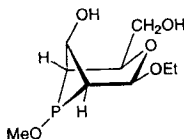
2-Carb-31.3. Bivalent and trivalent groups

The group formed by detaching one hydrogen atom from each of two (or three) carbon atoms of a monosaccharide is named by replacing the terminal 'e' of the monosaccharide name by '-diyl' (or '-triy!'), preceded by the appropriate locants.

Examples:



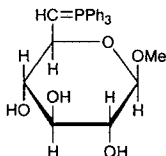
Methyl β -D-talopyranose-2-C,4-C-diylphosphinite
or 2-C,4-C-(methoxyphosphanediy!)- β -D-glucopyranose
or (2*R*,4*S*)-2-C,4-C-(methoxyphosphanediy!)- β -D-*threo*-hexopyranose



Methyl (ethyl 2,4-dideoxy- β -D-glucopyranoside-2,4-diylo)phosphinite
or ethyl 2,4-dideoxy-2,4-(methoxyphosphanediylo)- β -D-glucopyranoside

Residues formed by detaching two (or three) hydrogen atoms from the same carbon atom may be named similarly.

Example:



(Methyl 6-deoxy- β -D-glucopyranosid-6-ylidene)triphenyl- λ^5 -phosphane
or methyl 6-deoxy-6-triphenyl- λ^5 -phosphanylidene- β -D-glucopyranoside

Note. Names based on phosphane, rather than phosphine or phosphorane, are used in this document, as recommended in [14].

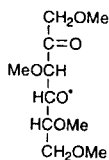
2-Carb-32. Radicals, cations and anions

Naming procedures described in this section follow the recommendations given in [25].

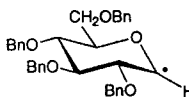
2-Carb-32.1. Radicals

Names for radicals are formed in the same way as those for the corresponding substituent groups (see 2-Carb-31.2).

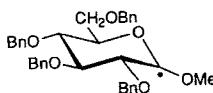
Examples:



1,3,5,6-Tetra-*O*-methyl-D-fructos-4-*O*-yl



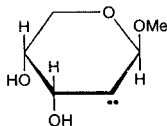
Tetra-*O*-benzyl-D-glucopyranosyl



2,3,4,6-Tetra-*O*-benzyl-1-methoxy-D-glucopyranosyl

Carbenes are named analogously by use of the suffix '-ylidene'.

Example:

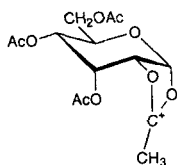
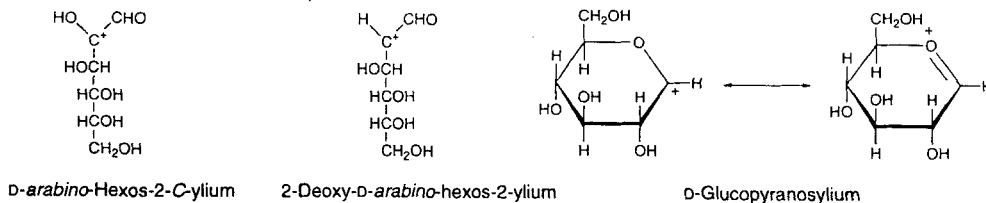


Methyl 2-deoxy- β -D-*erythro*-pentopyranosid-2-ylidene

2-Carb-32.2. Cations

Cations produced by formal loss of H⁻ from a carbon atom are denoted by replacing terminal 'e' with the suffix '-ylium', in conjunction with appropriate locants and a 'deoxy-' prefix if necessary (cf. 2-Carb-31.2).

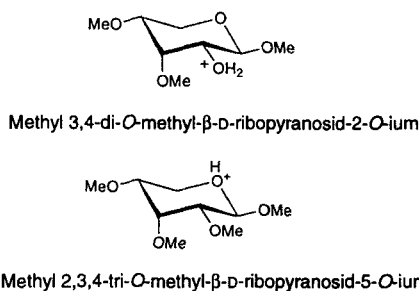
Examples:



3,4-Tri-O-acetyl-1,2-O-ethylidiumdiyl- α -D-allopyranose

Cations formed by hydration of an OH group or at the hemiacetal ring oxygen are denoted by the suffix '-O-ium', with numerical locant.

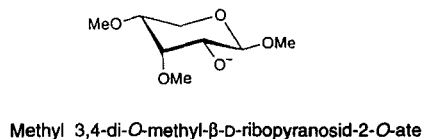
Examples:



2-Carb-32.3. Anions

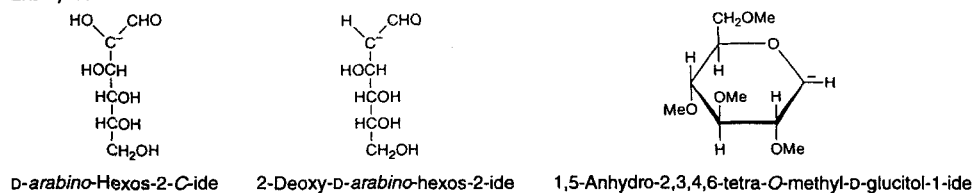
Anions produced by formal loss of H⁺ from an OH group are denoted by the suffix '-O-ate', with numerical locant.

Example:



Anions produced by formal loss of H⁺ from a carbon atom are denoted by the suffix '-ide', with appropriate locants and a 'deoxy-' prefix if necessary (cf. 2-Carb-31.2).

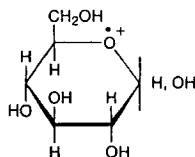
Examples:



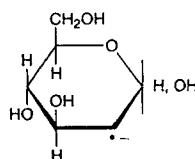
2-Carb-32.4. Radical ions

Radical ions can be named by adding the suffix 'yl' to ion names. Alternatively, the words 'radical cation' or 'radical anion' may be added after the name of the parent with the same molecular formula, especially when the location of the radical ion centre is not to be specified.

Examples:



D-Glucopyranosiumyl, or D-glucopyranose radical cation



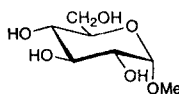
2-Deoxy-D-arabino-hexos-2-yl, or 2-deoxy-D-arabino-hexopyranos-2-ylidene radical anion

2-Carb-33. Glycosides and glycosyl compounds

2-Carb-33.1. Definitions

Glycosides were originally defined as mixed acetals (ketals) derived from cyclic forms of monosaccharides.

Example:



Methyl α -D-glucopyranoside

However, the term 'glycoside' was later extended to cover not only compounds in which, as above, the anomeric hydroxy group is replaced by a group $-OR$, but also those in which the replacing group is $-SR$ (thioglycosides), $-SeR$ (selenoglycosides), $-NR^1R^2$ (*N*-glycosides), or even $-CR^1R^2R^3$ (*C*-glycosides). 'Thioglycoside' and 'selenoglycoside' are legitimate generic terms; however the use of '*N*-glycoside', although widespread in biochemical literature, is improper and not recommended here ('glycosylamine' is a perfectly acceptable term). '*C*-Glycoside' is even less acceptable (see Note to 2-Carb-33.7). A glossary of terms based on 'glucose' is given in the Appendix.

Particularly in naturally occurring glycosides, the compound ROH from which the carbohydrate residue has been removed is often termed the aglycone, and the carbohydrate residue itself is sometimes referred to as the 'glycone'.

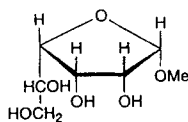
Note. The spelling 'aglycon' is often encountered.

2-Carb-33.2. Glycosides

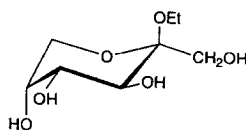
Glycosides can be named in three different ways:

(a) By replacing the terminal '-e' of the name of the corresponding cyclic form of the monosaccharide by '-ide' and preceding this, as a separate word (the intervening space is significant), the name of the group R (see examples below).

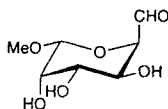
Examples:



Methyl α -D-gulofuranoside
not methyl- α -D-gulofuranoside



Ethyl β -D-fructopyranoside

Methyl (6*R*)-*D*-gluco-hexodialdo-6,2-pyranoside

Note. This is the 'classical' way of naming glycosides. It is used mainly when the group R is relatively simple (e.g. methyl, ethyl, phenyl).

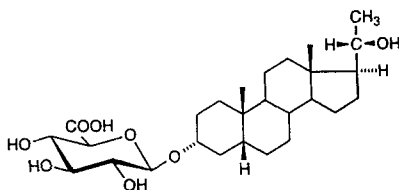
(b) By using the term 'glycosyloxy-', in the appropriate form for the monosaccharide, as prefix, for the name of the compound.

Note. This prefix includes the oxygen of the glycosidic bond. An example is given in 2-Carb-31.2; more are given below.

(c) By using the term '*O*-glycosyl-' as prefix to the name of the hydroxy compound.

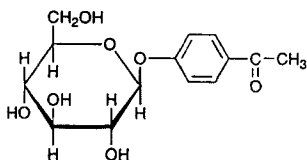
Note. This prefix does not include the oxygen of the glycosidic group. This is the appropriate method for naming natural products if the trivial name includes the OH group. The system is also used to name oligosaccharides (see 2-Carb-37).

Examples:

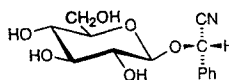


(20*S*)-20-Hydroxy-5β-pregnan-3α-yl β-*D*-glucopyranosiduronic acid
or (20*S*)-3α-(β-*D*-glucopyranosyloxyuronic acid)-5β-pregnan-20-ol;
for biochemical usage, pregnanediol 3-glucuronide

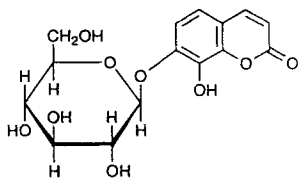
Note. A common biochemical practice would give the name (20*S*)-3α-(β-*D*-glucopyranuronosyloxy)-5β-pregnan-20-ol. This practice of naming glycosyl residues from uronic acids as 'glucuronosyl' is unsatisfactory because it implies the acceptance of the parent name 'glucuronose'. However the use of a two-word substituent prefix (glycosyloxyuronic acid), ending with a functional class name, remains inherently problematic, since it contravenes general organic nomenclature principles [13,14]. The latter practice has the advantage of retaining homomorphic relationships between glycoses and glycuronic acids.



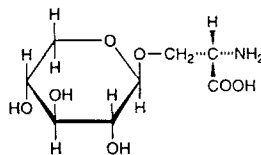
4-Acetylphenyl β-*D*-glucopyranoside
or 4'-(β-*D*-glucopyranosyloxy)acetophenone;
trivial name picein



(*S*)-*O*-β-*D*-Glucopyranosylmandelonitrile
or (*S*)-(β-*D*-glucopyranosyloxy)(phenyl)acetonitrile;
trivial name sambunigrin



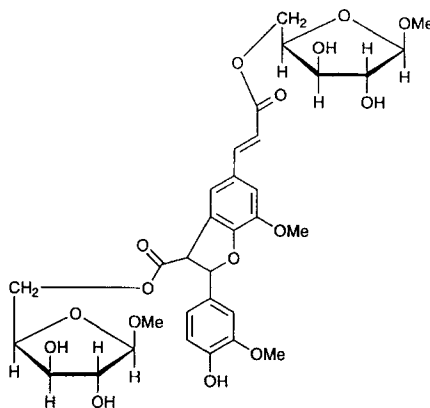
7-(β-*D*-Glucopyranosyloxy)-8-hydroxycoumarin;
trivial name daphnin



*O*³-β-*D*-Xylopyranosyl-*L*-serine [(*Xyl*-)*Ser*]

Glycosides can be named as substituents by the methods of 2-Carb-31.

Example:



(Methyl 5-deoxy- β -D-xylofuranosid-5-yl) 2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-5-[2-(methyl β -D-xylofuranosid-5-O-ylcarbonyl)vinyl]-2,3-dihydrobenzofuran-3-carboxylate

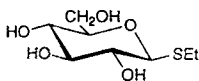
2-Carb-33.3. Thioglycosides

Names for individual compounds can be formed, like those for glycosides, in three ways, as follows.

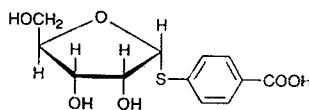
- By using the term thioglycoside, preceded by the name of the group R.
- With the prefix 'glycosylthio-', followed by the name of the compound RH; this prefix includes the sulfur atom.
- With the prefix 'S-glycosyl-' (not including the S atom), followed by the name of the thio compound.

Sulfoxides and sulfones can also be named by functional class nomenclature [13, 14].

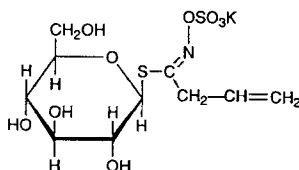
Examples:



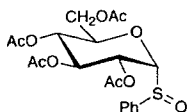
Ethyl 1-thio- β -D-glucopyranoside



4-(α -D-Ribofuranosylthio)benzoic acid
or 4-carboxyphenyl 1-thio- α -D-ribofuranoside



S- β -D-Glucopyranosyl (*Z*)-O-(potassium sulfonato)but-3-enehydroximothioate
(trivial name sinigrin)

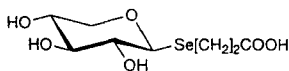


Phenyl tetra-*O*-acetyl- α -D-glucopyranosyl sulfoxide
or phenyl 2,3,4,6-tetra-*O*-acetyl-1-thio- α -D-glucopyranoside *S*-oxide

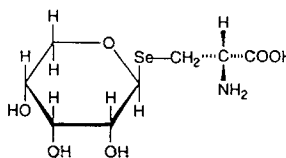
2-Carb-33.4. Selenoglycosides

Names are formed analogously to those for thioglycosides (2-Carb-33.3).

Examples:



2-Carboxyethyl 1-seleno-β-D-xylopyranoside
or 3-(β-D-xylopyranosylseleno)propanoic acid

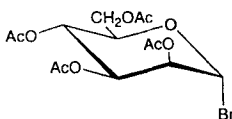


Se-β-D-Ribopyranosyl-D-selenocysteine
or (S)-2-amino-2-carboxyethyl 1-seleno-β-D-ribofuranoside
or 3-(β-D-ribofuranosylseleno)-D-alanine

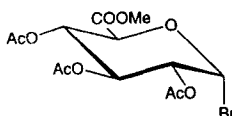
2-Carb-33.5. Glycosyl halides

Compounds in which the anomeric hydroxy group is replaced by a halogen atom are named as glycosyl halides. Pseudohalides (azides, thiocyanates etc.) are named similarly.

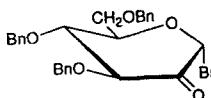
Examples:



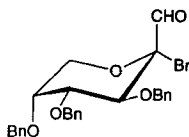
Tetra-O-acetyl-α-D-mannopyranosyl bromide



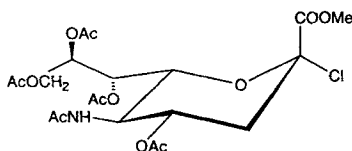
Methyl (2,3,4-tri-O-acetyl-α-D-glucopyranosyl)uronate bromide
not methyl 2,3,4-tri-O-acetyl-1-bromo-1-deoxy-α-D-glucopyranuronate



3,4,6-Tri-O-benzyl-α-D-arabino-hexopyranosyl-2-ulose bromide



3,4,5-Tri-O-benzyl-α-D-arabino-hexos-2-ulo-2,6-pyranosyl bromide
or 3,4,5-tri-O-benzyl-aldehydo-α-D-arabino-hexos-2-ulopyranosyl bromide

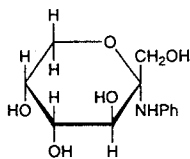


Methyl (5-acetamido-4,7,8,9-tetra-O-acetyl-3,5-dideoxy-D-glycero-α-D-galacto-non-2-ulopyranosyl)onate chloride

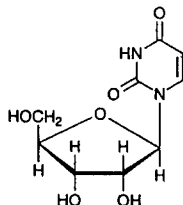
2-Carb-33.6. *N*-Glycosyl compounds (glycosylamines)

N-Glycosyl derivatives are conveniently named as glycosylamines. In the case of complex heterocyclic amines, such as nucleosides, the same approach is used.

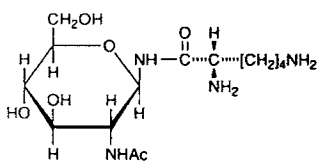
Examples:



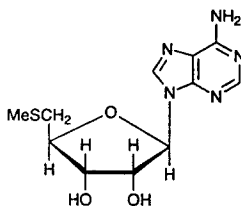
N-Phenyl- α -D-fructopyranosylamine
not aniline α -D-fructopyranoside



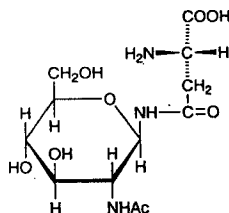
1- β -D-Ribofuranosyluracil (trivial name uridine)



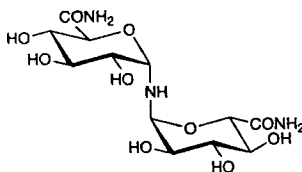
N^1 -(2-Acetamido-2-deoxy- β -D-glucopyranosyl)-L-lysynamide (Lys-NH-GlcNAc)
[trivial name N^1 -(*N*-acetylglucosaminy)-L-lysynamide]



9-(5-*S*-Methyl-5-thio- β -D-ribofuranosyl)adenine



N^4 -(2-Acetamido-2-deoxy- β -D-glucopyranosyl)-L-asparagine [(GlcNAc-)Asn]
or 2-acetamido- N^1 -L- β -aspartyl-2-deoxy- β -D-glucopyranosylamine
(trivial name β -*N*-acetylglucosaminy-L-asparagine)



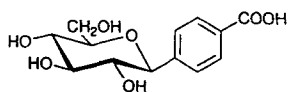
Bis(α -D-glucopyranosyluronamide)amine

2-Carb-33.7. C-Glycosyl compounds

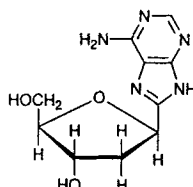
Compounds arising formally from the elimination of water from the glycosidic hydroxy group and an H atom bound to a carbon atom (thus creating a C-C bond) are named using the appropriate 'glycosyl-' prefixes (or other methods as appropriate, avoiding 'C-glycoside' terminology).

Note. The term *C-glycoside*, introduced for naming pseudouridine (a nucleoside from transfer RNA), is a misnomer. All other glycosides are hydrolysable; the C-C bond of '*C-glycosides*' is usually not. The use and propagation of names based on '*C-glycoside*' terminology is therefore strongly discouraged.

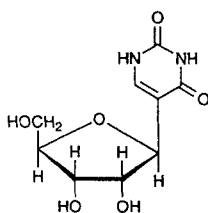
Example:



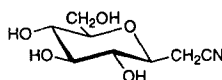
4- β -D-Glucopyranosylbenzoic acid
not 4-carboxyphenyl C- β -D-glucopyranoside



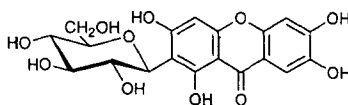
8-(2-Deoxy- β -D-*erythro*-pentofuranosyl)adenine
not adenine 8-(2-deoxyribose)



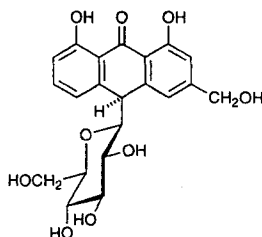
5- β -D-Ribofuranosyluracil; trivial name pseudouridine



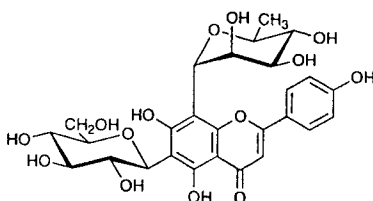
3,7-Anhydro-2-deoxy-D-*glycero*-D-*gulo*-octonitrile
or 2-C-(β -D-glucopyranosyl)acetonitrile
not cyanomethyl C- β -D-glucopyranoside



2- β -D-Glucopyranosyl-1,3,6,7-tetrahydroxanthren-9-one; trivial name mangiferin



(10*S*)-10- β -D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)anthracen-9(10*H*)-one;
trivial names aloin A, (10*S*)-barbaloin



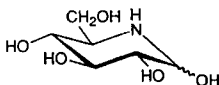
6- β -D-Glucopyranosyl-4',5,7-trihydroxy-8- α -L-rhamnopyranosylflavone; trivial name violanthin

2-Carb-34. Replacement of ring oxygen by other elements

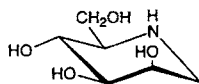
2-Carb-34.1. Replacement by nitrogen or phosphorus

Names should be based on those of the amino sugars (see 2-Carb-14) (or the analogous phosphanyl sugars) with the amino or phosphanyl group at the non-anomeric position. Ring-size designators (furano, pyrano etc.) are the same as for the oxygen analogues.

Examples:

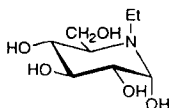


5-Amino-5-deoxy-D-glucopyranose; trivial name nojirimycin

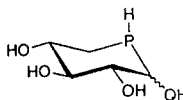


1-Amino-1,5-anhydro-1-deoxy-D-mannitol or 1,5-dideoxy-1,5-imino-D-mannitol;
trivial name deoxymannojirimycin

Note the extension of the use of 'anhydro' in the above example to include the elimination of water between $-\text{NH}_2$ and $-\text{OH}$ (cf. 2-Carb-26).

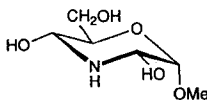


5-Deoxy-5-ethylamino- α -D-glucopyranose



5-Deoxy-5-phosphanyl-D-xylopyranose

Note. Use of the terms 'aza sugar', 'phospha sugar' etc. should be restricted to structures where carbon, not oxygen, is replaced by a heteroatom. Thus the structure below is a true aza sugar. The term 'imino sugar' may be used as a class name for cyclic sugar derivatives in which the ring oxygen atom has been replaced by nitrogen.



Methyl 3-deoxy-3-aza- α -D-ribo-hexopyranoside

2-Carb-34.2. Replacement by carbon

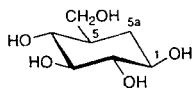
The (non-detachable) prefix 'carba-' signifies replacement of a heteroatom by carbon in general natural product nomenclature [26], and may be applied to replacement of the hemiacetal ring oxygen in carbohydrates if there is a desire to stress homomorphic relationships. If the original heteroatom is unnumbered, the new carbon atom is assigned the locant of the non-anomeric adjacent skeletal atom, with suffix 'a'.

Note. The draft natural product rules [26] recommend that the new carbon atom takes the locant of the *lower*-numbered proximal atom. However, carbohydrate chemists regard the ring oxygen as formally originating from the non-anomeric (usually *higher*-numbered) position.

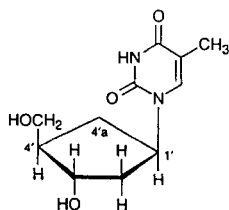
Additional stereochemistry (if any) at the new carbon centre is specified by use of the *R/S* system ([13], Section E).

Structures of this type can also be named as cyclitols [8].

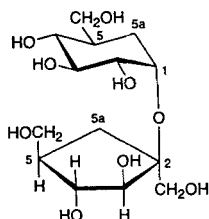
Examples:



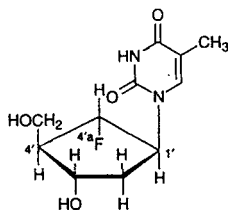
5a-Carba-β-D-glucopyranose



1-(2-Deoxy-4a-carba-β-D-*erythro*-pentofuranosyl)thymine
or 4'a-carbathymidine



5a-Carba-β-D-fructofuranosyl 5a-carba-α-D-glucopyranoside



1-[(4a*S*)-2-Deoxy-4a-fluoro-4a-carba-β-D-*erythro*-pentofuranosyl]thymine
or (4'a*S*)-4'a-fluoro-4'a-carbathymidine

2-Carb-35. Carbohydrates containing additional rings

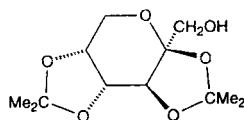
Internal bridging of carbohydrate structures by bivalent substituent groups creates additional rings, which can be named either by use of a substituent prefix representing the bridging group, or by fusion nomenclature. The following recommendations for the use of these two approaches are not thoroughly developed; they simply represent an attempt to rationalize and codify current literature practice in the use of systems not in general well suited to carbohydrate applications. Bridging substituent prefix nomenclature (2-Carb-35.1) is based on the system well established for simple cyclic acetals (2-Carb-28), and fusion nomenclature (2-Carb-35.2) on current literature usage and requirements for general natural product nomenclature [26].

2-Carb-35.1. Use of bivalent substituent prefixes

Where the new bridge is attached to oxygen (or a replacement heteroatom, e.g. nitrogen in an amino sugar) already indicated in the name of the unbridged carbohydrate, the bivalent substituent prefix denotes substitution at two heteroatoms as outlined in 2-Carb-24.1 and 2-Carb-25 [method (b)]. Heteroatoms not directly bonded to the carbohydrate chain are regarded as part of the bridge.

Where the new bridge is attached through C-C bonds to the carbohydrate chain, the bridge prefix denotes a double C-substitution. Procedures are as outlined in 2-Carb-16.

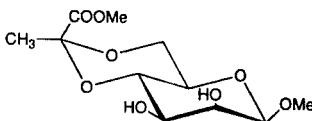
Examples:



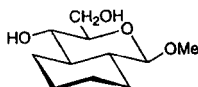
2,3:4,5-Di-O-isopropylidene- β -D-fructopyranose

Note 1. The alternative fusion name (see 2-Carb-35.2) is 2,2,2',2'-tetramethyl-4,4',5,5'-tetrahydro-(2,3,4,5-tetraoxo- β -D-fructopyranoso)[2,3-*d*:4,5-*d'*]bis[1,3]dioxole; this is clearly less desirable on grounds of complexity.

Note 2. The use of prefixes ending in '-ylidene' for *gem*-bivalent substituent groups is traditional in the carbohydrate field, although no longer recommended in general organic nomenclature [14].

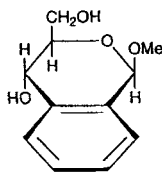


Methyl [(*S*)-4,6-O-(1-methoxycarbonyl)ethylidene]- β -D-mannopyranoside



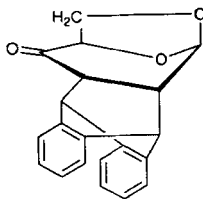
Methyl 2,3-(butane-1,4-diyl)-2,3-dideoxy- β -D-glucopyranoside

Note. The alternative fusion name (see 2-Carb-35.2) is hexahydro(methyl 2,3-dideoxy- β -D-glucopyranosido)[2,3]benzene

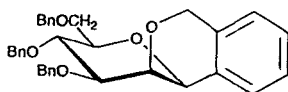


Methyl 2,3-(buta-1,3-diene-1,4-diyl)-2,3-dideoxy- β -D-*erythro*-hex-2-enopyranoside

Note. The alternative fusion name (see 2-Carb-35.2) is (methyl 2,3-dideoxy- β -D-*erythro*-hexopyranosido)[2,3]benzene



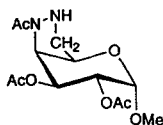
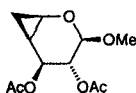
1,6-Anhydro-2,3-dideoxy-2,3-(9,10-dihydroanthracene-9,10-diyl)- β -D-*ribo*-hexopyranos-4-ulose

(1*S*)-1,5-Anhydro-3,4,6-tri-*O*-benzyl-1-*C*,2-*O*-(*o*-phenylenemethylene)-*D*-mannitol

Note. The isomeric chromene would be named as a 2-*O*,1-*C*-substituted system.

The prefix 'cyclo-' may be used for a single-bond bridge [14].

Examples:

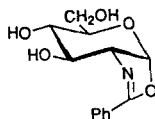
Methyl 4-*N*-acetyl-2,3-di-*O*-acetyl-4,6-diamino-4,6-*N*-cyclo-4,6-dideoxy- α -*D*-galactopyranosideMethyl 2,3-di-*O*-acetyl-4,6-cyclo-4,6-dideoxy- β -*D*-galactopyranoside

2-Carb-35.2. Ring fusion methods

Fusion methods are employed as in general natural product nomenclature [26], except that the original carbohydrate ring is cited first, in parentheses (with terminal '-e', if present, replaced by '-o'). For designating stereochemistry, bonds in the new ring are considered as equivalent to OH, unless OH (or its equivalent) is still present at the ring junction. Substituents on the carbohydrate portion are included within the parentheses enclosing the fusion prefix. Substituents on the new ring (including 'hydro-' prefixes) precede the carbohydrate term(s). If there is a choice, the new ring is numbered in the direction used to define the fusion locants.

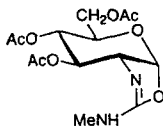
Note. General natural product fusion nomenclature [26] would require the carbohydrate portion to be cited last (e.g. oxazologlucopyranose), whereas it is cited first here and in the literature.

Examples:

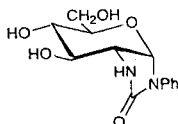
2-Phenyl-4,5-dihydro-(1,2-dideoxy- α -*D*-glucopyranoso)[2,1-*d*]-1,3-oxazole

Note 1. The alternative name using a substituent prefix (see 2-Carb-35.1) is 2-amino-1-*O*,2-*N*-(benzylidene)-2-deoxy- α -*D*-glucopyranose.

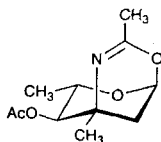
Note 2. Literature fusion names for this type of compound use 'glucopyrano[2,1-*d*]oxazoline' terminology. However, names for partially hydrogenated heterocycles ending in 'oline' were abandoned by IUPAC in 1983 [27], in favour of 'dihydro.....ole'. Use of 'pyranoso' rather than 'pyrano' is recommended to avoid confusion with the normal fusion prefix from 'pyran' and to simplify rules for naming derivatives (e.g. glycosides).

2-Methylamino-4,5-dihydro-(3,4,6-tri-*O*-acetyl-1,2-dideoxy- α -*D*-glucopyranoso)[2,1-*d*]-1,3-oxazole

Note. The alternative name using a substituent prefix (see 2-Carb-35.1) is 3,4,6-tri-*O*-acetyl-2-amino-2-deoxy-1-*O*,2-*N*-[(methylamino)methylidene]- α -*D*-glucopyranose.

3-Phenyltetrahydro-(1,2-dideoxy- α -D-glucopyranoso)[1,2-*d*]imidazol-2-one

Note. The alternative name using a substituent prefix (see 2-Carb-35.1) is 2-amino-1,2-*N*-carbonyl-1,2-dideoxy-1-*N*-phenyl- α -D-glucopyranosylamine

2-Methyl-5,6-dihydro-(4-*O*-acetyl-1,2,3,6-tetra-deoxy-3-methyl- α -L-ribo-hexopyranoso)[3,2,1-*de*]-4*H*-1,3-oxazine

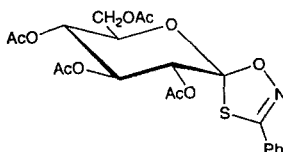
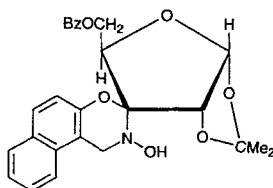
Note 1. The alternative name using a substituent prefix (see 2-Carb-35.1) is 4-*O*-acetyl-3-amino-2,3,6-trideoxy-1-*O*,3-*N*-(ethan-1-yl-1-ylidene)-3-*C*-methyl- α -L-ribo-hexopyranose

Note 2. This example would not normally be regarded as a fused system for nomenclature purposes, since it is not *ortho*- or *ortho*- and *peri*-fused [13].

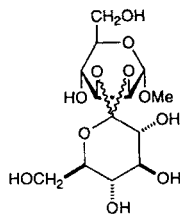
2-Carb-35.3. Spiro systems

Spiro systems can be named by normal procedures [13]. For clarity, any anhydro or deoxy prefixes or chalcogen replacement prefixes (e.g. thio) referring to the spiro junction should appear next to the carbohydrate stem. The carbohydrate component is cited first. Configuration at the spiro junction is assigned by the *R,S* system.

Example:

(1*R*)-2,3,4,6-Tetra-*O*-acetyl-3'-phenylspiro[1,5-anhydro-D-glucitol-1,5'-[1,4,2]oxathiazole](3*S*)-5-*O*-Benzoyl-1',2'-dihydro-1,2-*O*-isopropylidene-spiro[3-deoxy- α -D-*erythro*-pentofuranose-3,3'-naphtho[1,2-*e*][1,3]oxazin]-2'-ol

The following spiro disaccharide example is best named by use of a *gem*-bivalent substituent prefix:

Methyl 2,3-*O*-D-glucopyranosylidene- α -D-mannopyranoside

Stereochemistry at C-1 of the glucose residue could be indicated as *R* or *S*, e.g. [(1*R*)-2,3-*O*-D-glucopyranosylidene].....

2-Carb-36. Disaccharides

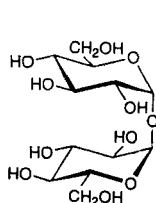
2-Carb-36.1. Definition

A disaccharide is a compound in which two monosaccharide units are joined by a glycosidic linkage.

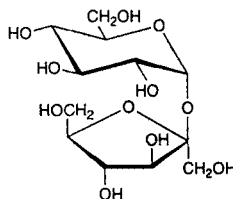
2-Carb-36.2. Disaccharides without a free hemiacetal group

Disaccharides which can be regarded as formed by reaction of the two glycosidic (anomeric) hydroxy groups with one another are named, systematically, as glycosyl glycosides. The parent (cited as the 'glycoside' component) is chosen according to 2-Carb-2.1. Both anomeric descriptors must be included in the name.

Examples:



α -D-Glucopyranosyl α -D-glucopyranoside
[α -D-Glcp-(1 \leftrightarrow 1)- α -D-Glcp]
(trivial name α,α -trehalose)

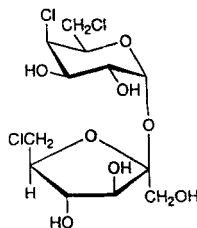


β -D-Fructofuranosyl α -D-glucopyranoside
[β -D-Fruf-(2 \leftrightarrow 1)- α -D-Glcp]
not α -D-glucopyranosyl β -D-fructofuranoside
(trivial names sucrose, saccharose)

Note. Such disaccharides are also known as non-reducing disaccharides.

If derivatives are named on the basis of the trivial name, the component cited first in the systematic name receives primed locants.

Example:



4,6,6'-Trichloro-4,6,6'-trideoxygalactosucrose
or 6-chloro-6-deoxy- β -D-fructofuranosyl 4,6-dichloro-4,6-dideoxy- α -D-galactopyranoside
(‘galactosucrose’ is a trivial name for the 4-epimer of sucrose)

2-Carb-36.3. Disaccharides with a free hemiacetal group

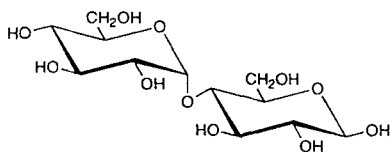
A disaccharide in which one glycosyl unit has replaced the hydrogen atom of an alcoholic hydroxy group of the other is named as a glycosylglycoside. The locants of the glycosidic linkage and the anomeric descriptor(s) must be given in the full name.

There are two established methods in use for citing locants: either in parentheses between the glycosyl and glycoside terms, or in front of the glycosyl prefix, as in the names of glycosides. The former (preferred) method is derived from that used to designate residues in oligosaccharides (see 2-Carb-37 and -38).

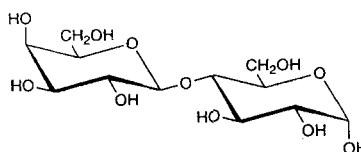
Note. The latter method is that used by Chemical Abstracts Service for disaccharides.

The *O*-locants used for the former method in the previous recommendations [1] are omitted here.

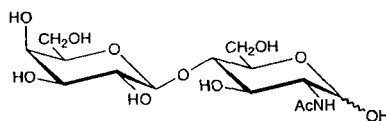
Examples:



β -D-Glucopyranosyl-(1 \rightarrow 4)- β -D-glucopyranose
 $[\alpha$ -D-Glcp-(1 \rightarrow 4)- β -D-Glcp]
 or 4-*O*- α -D-glucopyranosyl- β -D-glucopyranose
 (trivial name β -maltose, not β -D-maltose)



β -D-Galactopyranosyl-(1 \rightarrow 4)- α -D-glucopyranose
 $[\beta$ -D-Galp-(1 \rightarrow 4)- α -D-Glcp]
 or 4-*O*- β -D-galactopyranosyl- α -D-glucopyranose
 (trivial name α -lactose, not α -D-lactose)



β -D-Galactopyranosyl-(1 \rightarrow 4)-*N*-acetyl-D-glucosamine (trivial name *N*-acetyllactosamine; LacNAc)

Note. Disaccharides with a free hemiacetal group are also known as reducing disaccharides.

2-Carb-36.4 Trivial names

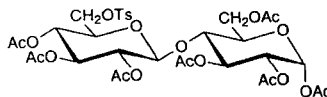
Many of the naturally occurring disaccharides have well established trivial names. Some of these are listed below, together with the systematic names in both versions (see above).

Cellobiose	β -D-Glucopyranosyl-(1 \rightarrow 4)-D-glucose 4- <i>O</i> - β -D-Glucopyranosyl-D-glucose
Gentiobiose	β -D-Glucopyranosyl-(1 \rightarrow 6)-D-glucose 6- <i>O</i> - β -D-Glucopyranosyl-D-glucose
Isomaltose	α -D-Glucopyranosyl-(1 \rightarrow 6)-D-glucose 6- <i>O</i> - α -D-Glucopyranosyl-D-glucose
Melibiose	α -D-Galactopyranosyl-(1 \rightarrow 6)-D-glucose 6- <i>O</i> - α -D-Galactopyranosyl-D-glucose
Primeverose	β -D-Xylopyranosyl-(1 \rightarrow 6)-D-glucose 6- <i>O</i> - β -D-Xylopyranosyl-D-glucose
Rutinose	α -L-Rhamnopyranosyl-(1 \rightarrow 6)-D-glucose 6- <i>O</i> - α -L-Rhamnopyranosyl-D-glucose

The systematic names of trehalose, sucrose, maltose and lactose have been given already (with the formulae).

If derivatives are named on the basis of the trivial name, the component cited first in the systematic name receives primed locants.

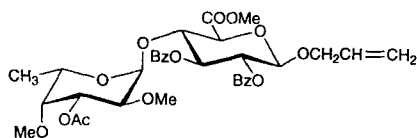
Example:



1,2,2',3,3',4',6-Hepta-*O*-acetyl-6'-*O*-tosyl- α -cellobiose
 or 2,3,4-tri-*O*-acetyl-6-*O*-tosyl- β -D-glucopyranosyl-(1 \rightarrow 4)-1,2,3,6-tetra-*O*-acetyl- α -D-glucopyranose

If the reducing terminal is a uronic ester glycoside, the ester alkyl group is cited at the beginning of the name, and the aglyconic alkyl group is cited with the name of the glycosidic residue.

Example:



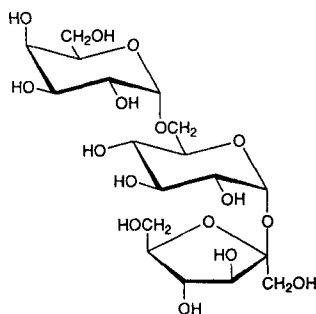
Methyl (3-*O*-acetyl-6-deoxy-2,4-di-*O*-methyl- α -L-galactopyranosyl)-(1 \rightarrow 4)-(allyl 2,3-di-*O*-benzoyl- β -D-glucopyranosid)uronate

2-Carb-37. Higher oligosaccharides

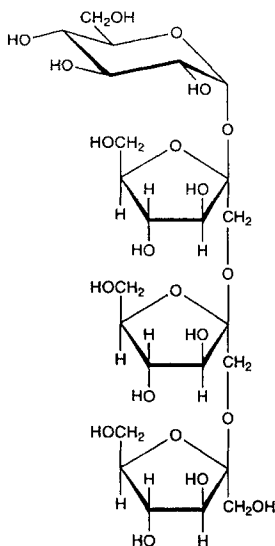
2-Carb-37.1. Oligosaccharides without a free hemiacetal group

Trisaccharides (for example) are named as glycosylglycosyl glycosides or glycosyl glycosylglycosides as appropriate. A choice between the two residues linked through their anomeric positions for citation as the 'glycoside' portion can be made on the basis of 2-Carb-2.1. Alternatively, a sequential (end-to-end) naming approach may be used, regardless of 2-Carb-2.1. The names are formed by the preferred method of naming disaccharides (see 2-Carb-36.3): the locant of the anomeric carbon atom, an arrow, and the locant of the connecting oxygen of the next monosaccharide unit are set in parentheses between the names of the residues concerned.

Examples:



β -D-Fructofuranosyl α -D-galactopyranosyl-(1 \rightarrow 6)- α -D-glucopyranoside
(glucose preferred to fructose for citation as 'glycoside')
or α -D-galactopyranosyl-(1 \rightarrow 6)- α -D-glucopyranosyl β -D-fructofuranoside
(sequential method)
[α -D-Galp-(1 \rightarrow 6)- α -D-Glcp-(1 \leftrightarrow 2) β -D-Fruf]
(trivial name raffinose)



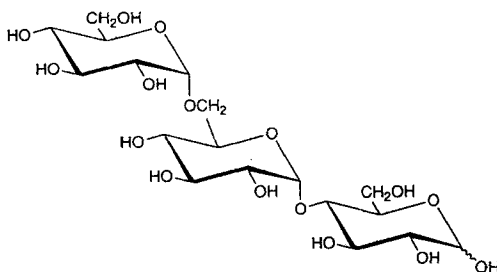
β -D-Fructofuranosyl-(2 \rightarrow 1)- β -D-fructofuranosyl-(2 \rightarrow 1)- β -D-fructofuranosyl α -D-glucopyranoside
 [β -D-Fruf(2 \rightarrow 1)- β -D-Fruf(2 \rightarrow 1)- β -D-Fruf(2 \leftrightarrow 1)- α -D-Glcp] (trivial name nystose)

If derivatives are to be named on the basis of the trivial name, the component cited last in the systematic name receives locants with no primes, the preceding component singly-primed locants, etc. However, naming of trisaccharide and higher oligosaccharide derivatives systematically is preferred, to avoid ambiguity.

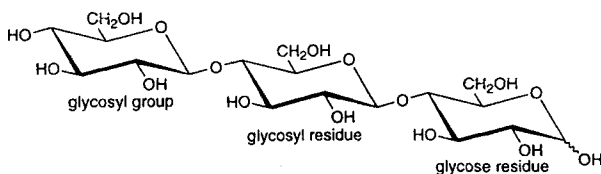
2-Carb-37.2. Oligosaccharides with a free hemiacetal group

An oligosaccharide of this class is named as a glycosyl[glycosyl]_nglycose, i.e. the reducing sugar is the parent. Anomeric descriptors and locants are given as described in 2-Carb-37.1. The conventional depiction has the reducing sugar (glycose residue) on the right and the non-reducing end (glycosyl group) on the left. Internal sugar units are called glycosyl residues (the term 'anhydrosugar unit' is misleading and its use is discouraged). As the reducing end is often converted into the corresponding alditol, aldonic acid or glycoside derivative, the more general term 'downstream end' has been proposed for this end of the molecule.

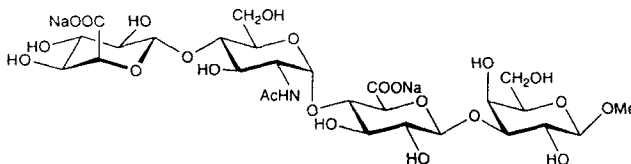
Examples:



α -D-Glucopyranosyl-(1 \rightarrow 6)- α -D-glucopyranosyl-(1 \rightarrow 4)-D-glucopyranose (trivial name panose)



β -D-Glucopyranosyl-(1 \rightarrow 4)- β -D-glucopyranosyl-(1 \rightarrow 4)-D-glucopyranose (trivial name cellotriose)

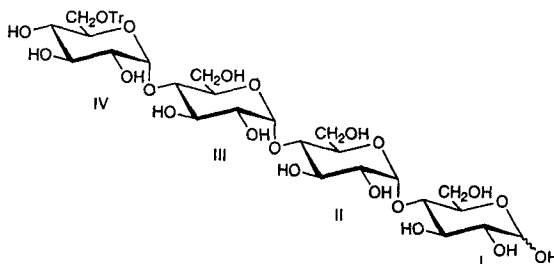


Methyl (sodium α -L-idopyranosyluronate)-(1 \rightarrow 4)-(2-acetamido-2-deoxy- α -D-glucopyranosyl)-(1 \rightarrow 4)-(sodium β -D-glucopyranosyluronate)-(1 \rightarrow 3)- β -D-galactopyranoside
{Na₂[α -L-IdoPA-(1 \rightarrow 4)- α -D-GlcpNAc-(1 \rightarrow 4)- β -D-GlcpA-(1 \rightarrow 3)- β -D-GalpOMe]}

Higher oligosaccharides are named systematically in the same way. However, it is often preferable to give their structures by use of the symbolic approach outlined in 2-Carb-38).

Trivial names for linear oligosaccharides consisting only of 1 \rightarrow 4 linked α -D-glucopyranosyl residues are maltotriose, maltotetraose etc. Similar names, based on the component sugar, are convenient for referring to other homo-oligosaccharides (e.g. xylobiose, galactotetraose), but such names should be used sparingly. Locants for naming substituted derivatives may be obtained by assigning roman numerals to the residues in ascending order starting from the reducing end.

Example:



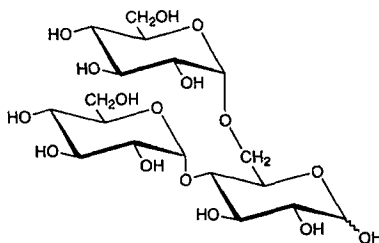
6^{IV}-O-Tritylmaltotetraose

Arabic numerals have also been used in this context, but confusion may result when component sugar residues have structural modifications (e.g. chain branches) requiring superscript locant numbers. The present recommendation follows long-established usage in glycolipids [21].

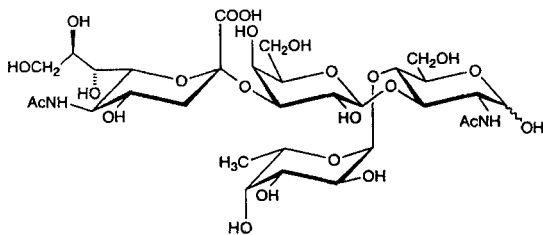
2-Carb-37.3. Branched oligosaccharides

Terms designating branches should be enclosed in square brackets. In a branched chain, the longest chain is regarded as the parent. If two chains are of equal length the one with lower locants at the branch point is preferred, although some oligosaccharides are traditionally depicted otherwise, such as the blood group A trisaccharide exemplified below.

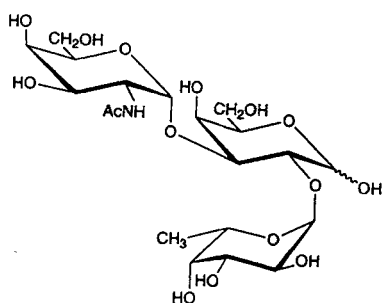
Examples:



α -D-Glucopyranosyl-(1 \rightarrow 4)-[α -D-glucopyranosyl-(1 \rightarrow 6)]-D-glucopyranose
[or 4,6-di-O-(α -D-glucopyranosyl)-D-glucopyranose]
(trivial name isopanose)



(5-Acetamido-3,5-dideoxy-D-glycero- α -D-galacto-non-2-ulopyranosylonic acid)-(2 \rightarrow 3)- β -D-galactopyranosyl-(1 \rightarrow 3)- $[\alpha$ -L-fucopyranosyl-(1 \rightarrow 4)]-2-acetamido-2-deoxy-D-glucopyranose
 or 5-N-acetyl- α -neuraminyI-(2 \rightarrow 3)- β -D-galactopyranosyl-(1 \rightarrow 3)- $[\alpha$ -L-fucopyranosyl-(1 \rightarrow 4)]-2-acetamido-2-deoxy-D-glucopyranose
 (α -Neup5Ac-(2 \rightarrow 3)- β -D-Galp-(1 \rightarrow 3)- $[\alpha$ -L-Fucp-(1 \rightarrow 4)]-D-GlcpNAc) (sialyl-Le^a trisaccharide)



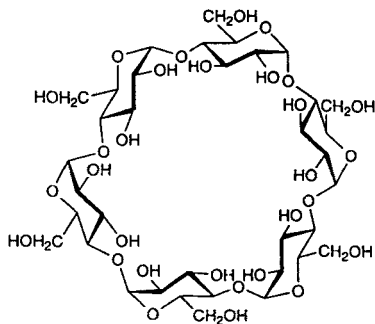
2-Acetamido-2-deoxy- α -D-galactopyranosyl-(1 \rightarrow 3)- $[\alpha$ -L-fucopyranosyl-(1 \rightarrow 2)]-D-galactopyranose
 (α -D-GalpNAc-(1 \rightarrow 3)- $[\alpha$ -L-Fucp-(1 \rightarrow 2)]-D-Galp) (blood group A trisaccharide)

2-Carb-37.4. Cyclic oligosaccharides

37.4.1. Semisystematic names

Cyclic oligosaccharides composed of a single type of oligosaccharide unit may be named semisystematically by citing the prefix 'cyclo', followed by terms indicating the type of linkage [e.g. 'malto' for α -(1 \rightarrow 4)-linked glucose units], the number of units (e.g. 'hexa' for six) and the termination '-ose'. The trivial names α -cyclodextrin (α -CD) for cyclomaltohexaose, β -cyclodextrin (β -CD) for cyclomaltoheptaose and γ -cyclodextrin (γ -CD) for cyclomaltooctaose are well established.

Example:



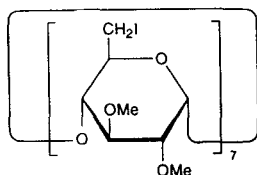
Cyclomaltohexaose (α -cyclodextrin, α -CD)

Structures with linkages other than (1→4) should be named systematically (see 2-Carb-37.4.2).

Note. The cyclic oligosaccharides arising from enzymic transglycosylation of starch have been referred to as Schardinger dextrins. These names (and those of the cyclohexaamylose type) are not recommended, but the abbreviation CD is tolerated.

Derivatives with the same substitution pattern on each residue can be named semisystematically by assigning a single multiplicative prefix (e.g. hexakis, heptakis etc.) to the substituent prefixes as a group.

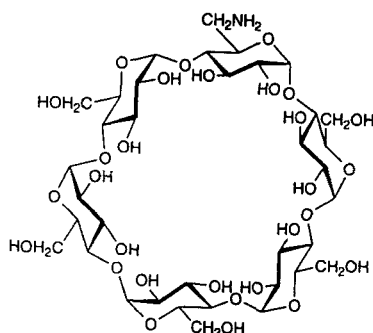
Example:



Heptakis(6-deoxy-6-iodo-2,3-di-O-methyl)cyclomaltoheptaose

Derivatives with different substitution patterns on the various residues can be named by the method of 2-Carb-37.2, assigning a roman numeral to each residue.

Example:

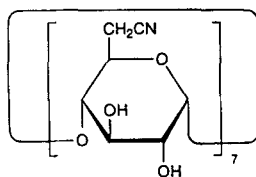


6'-Amino-6'-deoxycyclomaltohexaose

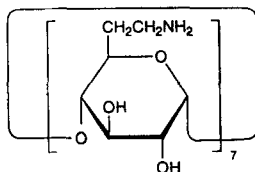
37.4.2. Systematic names

Cyclic oligosaccharides composed of a single type of residue can be named by giving the systematic name of the glycosyl residue, preceded by the linkage type in parentheses, preceded in turn by 'cyclo-' with a multiplicative suffix (i.e. 'cyclohexakis-' etc.)

Examples:



Cycloheptakis-(1→4)-(6-deoxy- α -D-glucopyranosylurononitrile)



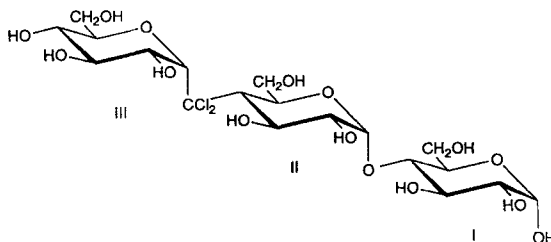
Cycloheptakis-(1→4)-(7-amino-6,7-dideoxy- α -D-glucopyranosyl)

The 1→6 isomer of cyclomaltohexaose should be named cyclohexakis-(1→6)- α -D-glucosyl, rather than cycloisomaltohexaose.

2-Carb-37.5. Oligosaccharide analogues

Structures in which the linking glycosidic oxygen is replaced by $-\text{CH}_2-$ may be named by use of the replacement prefix 'carba-' (cf. 2-Carb-34.2) for emphasis of homomorphic relationships. The oxygen replaced is given the locant of the carbon atom to which it is attached in the residue with the lower roman numeral (cited as superscript) (cf. 2-Carb-37.2), with suffix 'a'.

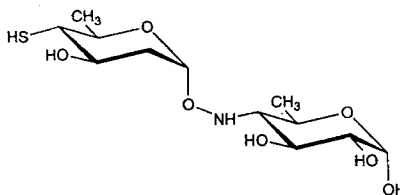
Example:



4''_a,4''_a-Dichloro-4''_a-carba- α -maltotriose

If the glycosidic oxygen link is replaced by $-\text{O}-\text{NH}-$, normal amino sugar nomenclature can be employed.

Example:



4-(2,6-Dideoxy-4-thio- α -D-arabino-hexopyranosyloxyamino)-4,6-dideoxy- α -D-glucopyranose

2-Carb-38. Use of symbols for defining oligosaccharide structures*

2-Carb-38.1. General considerations

Oligosaccharide and polysaccharide structures occur not only in free form but often as parts of glycopeptides or glycoproteins [11] or of glycolipids [21]. It can be cumbersome to designate their structures by using the recommendations of 2-Carb-37. The use of three-letter symbols for monosaccharide residues is therefore recommended. With appropriate locants and anomeric descriptors, long sequences can thus be adequately described in abbreviated form.

Symbols for the common monosaccharide residues and derivatives are listed in Table 2. They are generally derived from the corresponding trivial names. Abbreviations for substituents (see 2-Carb-1.16.2), preceded by locants, follow the monosaccharide abbreviations directly.

2-Carb-38.2. Representations of sugar chains

For writing the structure of an oligo- or poly-saccharide chain, the glucose residue [the 'reducing group', i.e. the residue with the free hemiacetal group or modification thereof (e.g. alditol, aldonic acid, glycoside)] should be at the right-hand end. Also, when there is a glycosyl linkage to a non-carbohydrate moiety (e.g. protein, peptide or lipid) the glycosyl residue involved should appear at the right.

Numbering of monosaccharide units, if desired, should proceed from right to left.

2-Carb-38.3. The extended form

This is the form employed by the carbohydrate databank CarbBank, and is preferred for most purposes. Each symbol for a monosaccharide unit is preceded by the anomeric descriptor and the configuration symbol. The

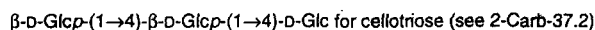
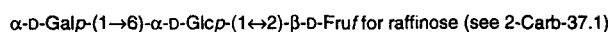
* The recommendations presented here are a modified version of the published 1980 recommendations [6].

Table 2. Symbols for monosaccharide residues and derivatives in oligosaccharide chains

Abequose	Abe	Iduronic acid	IdoA
Allose	All	Lyxose	Lyx
Altrose	Alt	Mannose	Man
Apiose	Api	Muramic acid	Mur
Arabinose	Ara	Neuraminic acid	Neu
Arabinitol	Ara-ol	<i>N</i> -Acetylneuraminic acid	Neu5Ac
2-Deoxyribose	dRib	<i>N</i> -Acetyl-2-deoxyneur-2-enaminic acid	Neu2en5Ac
Fructose	Fru	<i>N</i> -Glycolylneuraminic acid	Neu5Gc
Fucose	Fuc	3-Deoxy- <i>D</i> -manno-oct-2-ulosonic acid	Kdo
Fucitol	Fuc-ol	Rhamnose	Rha
Galactose	Gal	3,4-Di- <i>O</i> -methylrhamnose	Rha3,4Me2
Galactosamine	GalN	Psicose	Psi
<i>N</i> -Acetylgalactosamine	GalNAc	Quinovose	Qui
β - <i>D</i> -Galactopyranose 4-sulfate	β - <i>D</i> -Galp4S	Ribose	Rib
Glucose	Glc	Ribose 5-phosphate	Rib5P
Glucosamine	GlcN	Ribulose	Ribu (or Rul)
2,3-Diamino-2,3-dideoxy- <i>D</i> -glucose	GlcN3N	Sorbose	Sor
Glucitol	Glc-ol	Tagatose	Tag
<i>N</i> -Acetylglucosamine	GlcNAc	Talose	Tal
Glucuronic acid	GlcA	Xylose	Xyl
Ethyl glucopyranuronate	GlcP6Et	Xylulose	Xylul (or Xul)
Gulose	Gul	2- <i>C</i> -Methylxylose	Xyl2CMe
Idose	Ido		

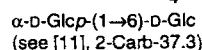
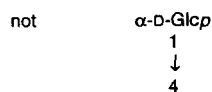
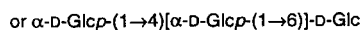
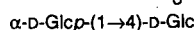
ring size is indicated by an italic *f* for furanose or *p* for pyranose, etc. The locants of the linkage are given in parentheses between the symbols; a double-headed arrow indicates a linkage between two anomeric positions. In Carbohydrate Bank, omission of α/β , *D/L*, or *f/p* means that this structural detail is not known.

Examples:



Branches are written on a second line, or in brackets on the same line.

Example:



for 4,6-Di-*O*- α -*D*-glucopyranosyl-*D*-glucose

The hyphens may be omitted, except that separating the configurational symbol and the three-letter symbol for the monosaccharide.

2-Carb-38.4. The condensed form

In the condensed form, the configurational symbol and the letter denoting ring size are omitted. It is understood that the configuration is D (with the exception of fucose and iduronic acid which are usually L) and that the rings are in pyranose form unless otherwise specified. The anomeric descriptor is written in the parentheses with the locants.

Example:

Gal(α 1-6)Glc(α 1-2 β)Fru for raffinose

For most purposes, the short form (2-Carb-38.5) is preferred when abbreviation of the extended form is desirable.

2-Carb-38.5. The short form

For longer sequences, it is desirable to shorten the notation even further by omitting (i) locants of anomeric carbon atoms, (ii) the parentheses around the locants of the linkage and (iii) hyphens (if desired). Branches can be indicated on the same line by using appropriate enclosing marks (parentheses, square brackets etc.). Whenever necessary, configuration symbols and ring size designators etc. may be included, to make the notation more specific.

Example:

Gal α -6Glc α - β Fru or Gal α 6Glc α β Fru for raffinose

The following examples show all three representations of the same structure:

(a) extended form

β -D-Galp-(1 \rightarrow 4)- β -D-Glc ρ NAC-(1 \rightarrow 2)- α -D-Man ρ -(1 \rightarrow



(b) condensed form in two lines

Gal(β 1-4)GlcNAC(β 1-2)Man(α 1-
|
Fuc(α 1-3)

or in one line

Gal(β 1-4)[Fuc(α 1-3)]GlcNAC(β 1-2)Man(α 1-

(c) short form

Gal β -4(Fuc α -3)GlcNAC β -2Man α -
or Gal β 4(Fuc α 3)GlcNAC β 2Man α -
or Gal β 4GlcNAC β 2Man α -
|
Fuc α 3

This last version is recommended as the most explicit representation of branching using the short form.

Note. These representations do not follow the recommendations for choice of main chain given in 2-Carb-37.3. Such deviations are common in depicting series of naturally occurring oligosaccharides where it is desirable to show homomorphic relationships.

2-Carb-39. Polysaccharides***2-Carb-39.1. Names for homopolysaccharides**

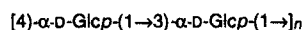
A general term for a polysaccharide (glycan) composed of a single type of monosaccharide residue is obtained by replacing the ending '-ose' of the sugar name by '-an'.

Note. Examples of established usage of the '-an' ending are: xylan for polymers of xylose, mannan for polymers of mannose, and galactan for polymers of galactose. Cellulose and starch are both glucans, as they are composed of glucose residues.

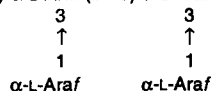
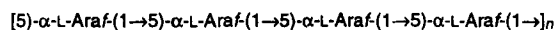
2-Carb-39.2. Designation of configuration of residues

When the configurational series of the monomer residues is known, D- or L- may be included as a prefix to the name.

Examples:



A D-glucan (nigeran)

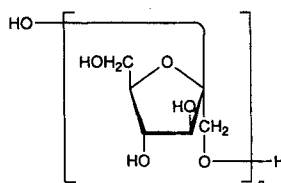


An L-arabinan (more specifically an α-L-arabinan)

2-Carb-39.3. Designation of linkage

When the major linkage in a homopolysaccharide is known, it may be indicated in the name. The linkage designation shows the carbon atoms involved in the glycosidic bonds. When specific sugars are designated, notation for glycosidic linkages should precede the symbols designating the configuration of the sugar; thus, (1→4)-α-D-glucan.

Examples:



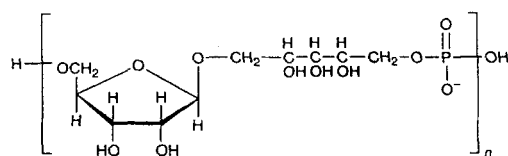
(2→1)-β-D-Fructofuranan (inulin has this structure, with a terminal α-D-glucopyranosyl group)



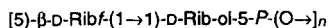
(1→4)-α-D-Glucopyranan (amylose)

Note. When the linkage between monosaccharide units is non-glycosidic (as in the phosphate derivative shown below), use of the glycan terminology is inappropriate; other methods of polymer nomenclature should be employed [20].

* This is a modified version of the 1980 recommendations on polysaccharide nomenclature [7].



Poly[(β-D-ribofuranosyl-5-O-yl)(1-deoxy-D-ribitol-1-C,5-O-diyl)(oxidophosphoryl)]



Such structures do not conform to the original strict definition of 'polysaccharide' but are generally classified as polysaccharides in current practice.

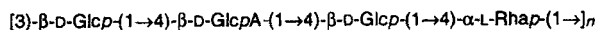
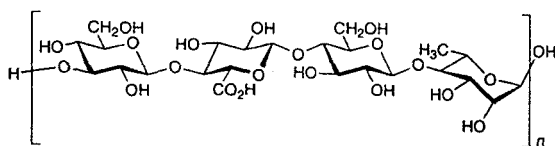
2-Carb-39.4. Naming of newly discovered polysaccharides

Names assigned to newly discovered polysaccharides should end in '-an'.

Examples:



Pustulan (a glucan from the lichen *Umbilicaria pustulata*)



Gellan (a bacterial polysaccharide originally designated S-60)

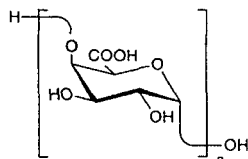
Note. The name ending in '-an' refers to the unsubstituted polysaccharide. Thus xylan occurs in nature in unacetylated and partially acetylated forms. Xylan designates the unacetylated material, and xylan acetate an acetylated derivative.

Well established names such as cellulose, starch, inulin, chitin, amylose and amylopectin are retained. 'Carrageenan' and 'laminaran' are now often used rather than the older names ending in '-in'.

2-Carb-39.5. Uronic acid derivatives.

A polysaccharide (glycan) composed entirely of glycuronic acid residues is named by replacing '-ic acid' by '-an'. The generic name for this group of polysaccharides is 'glycuronan'.

Example:

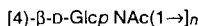


Note. The term glycuronan is used instead of 'polyuronide'; the latter term is incorrect.

2-Carb-39.6. Amino sugar derivatives

A polysaccharide composed entirely of amino sugar residues is named by appropriate modification of the systematic amino sugar name.

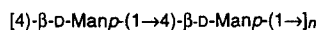
Example:



2-Carb-39.7. Polysaccharides composed of more than one kind of residue

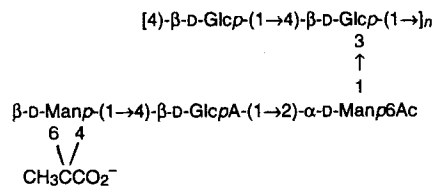
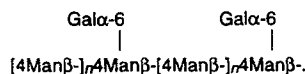
A heteropolysaccharide (heteroglycan) is a polymer containing two or more kinds of sugar (glucose) or modified sugar (e.g. aminodeoxyglyucose or glycuronic acid) residue. When the polysaccharide has a principal chain ('backbone') composed of only one type of sugar residue, this residue should be cited last (as a 'glycan' term), and the other types of residue cited as 'glyco-' prefixes in alphabetical order. However, when no single type of sugar residue constitutes the principal chain, all sugar residues should be cited alphabetically as 'glyco-' prefixes, and the name should terminate with the suffix '-glycan'.

Examples:



A D-galacto-D-mannan (guaran)

Note. A less branched D-galacto-D-mannan could be shown in the short form as:

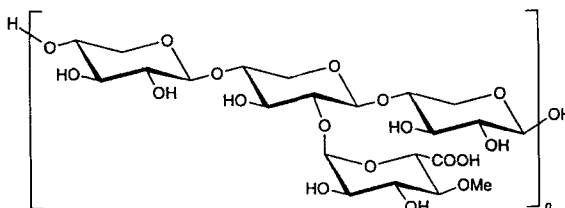


Xanthan

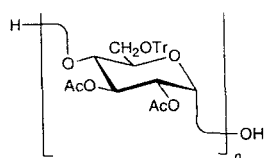
2-Carb-39.8. Substituted residues

When substitution occurs in a polysaccharide (glycan), each type of substituent is cited in the name at an appropriate position (in alphabetical order).

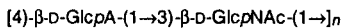
Examples:



(4-O-Methyl-α-D-glucurono)-D-xylan



2,3-Di-O-acetyl-6-O-tritylamylose



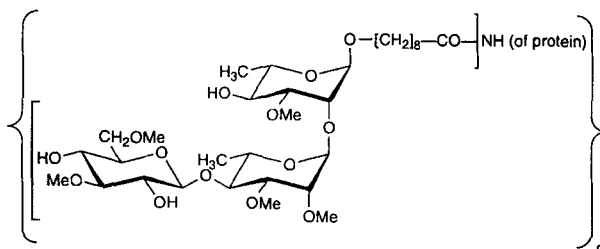
(2-Acetamido-2-deoxy-D-gluco)-D-glucuronoglycan (hyaluronic acid or hyaluronan)

2-Carb-39.9. Glycoproteins, glycopeptides and peptidoglycans

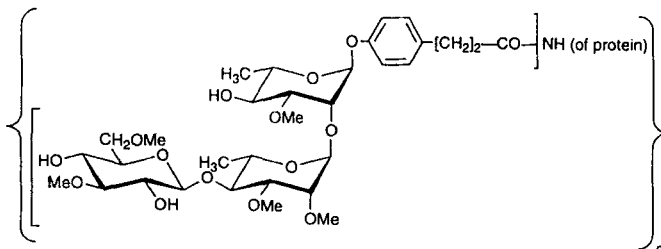
Polymers containing covalently bound monosaccharide and amino-acid residues are termed glycoproteins, glycopeptides or peptidoglycans. It is not possible to give precise distinctions between these terms. In general, glycoproteins are conjugated proteins containing either oligosaccharide groups or polysaccharide groups having a fairly low relative molecular mass. Proteoglycans are proteins linked to polysaccharides of high molecular mass. Peptidoglycans consist of polysaccharide chains covalently linked to peptide chains. The nomenclature of these compounds is discussed in [11].

Synthetically produced or modified carbohydrate-protein conjugates are sometimes referred to as neoglycoproteins. The nomenclature for the carbohydrate-containing substituents in such structures is analogous to sequential oligosaccharide nomenclature (2-Carb-37.2)

Examples:



Poly-[(3,6-Di-O-methyl- β -D-glucopyranosyl)-(1 \rightarrow 4)-(2,3-di-O-methyl- α -L-rhamnopyranosyl)-(1 \rightarrow 2)-(3-O-methyl- α -L-rhamnopyranosyloxy)-(1-O \rightarrow 9)-nonanoyl-(1 \rightarrow N)]-protein
 ([(β -D-Glcp3,6Me₂-(1 \rightarrow 4)- α -L-Rhap2,3Me₂-(1 \rightarrow 2)- α -L-Rhap3Me-(1-O \rightarrow 9)-nonanoyl-(1 \rightarrow N)]_nprotein)



Poly-[(3,6-Di-O-methyl- β -D-glucopyranosyl)-(1 \rightarrow 4)-(2,3-di-O-methyl- α -L-rhamnopyranosyl)-(1 \rightarrow 2)-(3-O-methyl- α -L-rhamnopyranosyloxy)-(1-O \rightarrow 4)-(3-phenylpropanoyl)-(1 \rightarrow N^{Lys})]-protein

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APPENDIX

Trivial Names for Carbohydrates and Derivatives
with their Systematic Equivalents and Symbols
(non-limiting list)

(a) parent monosaccharides

Allose (AlI)	<i>allo</i> -Hexose
Altrose (Alt)	<i>altro</i> -Hexose
Arabinose (Ara)	<i>arabino</i> -Pentose
Erythrose	<i>erythro</i> -Tetrose
Erythrulose	<i>glycero</i> -Tetrolose
Fructose (Fru)	<i>arabino</i> -Hex-2-ulose
D-Fucitol (D-Fuc-ol)	6-Deoxy-D-galactitol
L-Fucitol (L-Fuc-ol)	1-Deoxy-D-galactitol
Fucosamine (FucN)	2-Amino-2,6-dideoxygalactose
Fucose (Fuc)	6-Deoxygalactose
Galactosamine (GalN)	2-Amino-2-deoxygalactose
D-Galactosaminitol (GalN-ol)	2-Amino-2-deoxy-D-galactitol
Galactose (Gal)	<i>galacto</i> -Hexose
Glucosamine (GlcN)	2-Amino-2-deoxyglucose
Glucosaminitol (GlcN-ol)	2-Amino-2-deoxyglucitol
Glucose (Glc)	<i>gluco</i> -Hexose
Glyceraldehyde	2,3-Dihydroxypropanal
Glycerol (Gro)	Propane-1,2,3-triol
Glycerone (1,3-dihydroxyacetone)	1,3-Dihydroxypropanone
Gulose (Gul)	<i>gulo</i> -Hexose
Idose (Ido)	<i>ido</i> -Hexose
Lyxose (Lyx)	<i>lyxo</i> -Pentose
Mannosamine (ManN)	2-Amino-2-deoxymannose
Mannose (Man)	<i>manno</i> -Hexose
Psicose (Psi)	<i>ribo</i> -Hex-2-ulose
Quinovose (Qui)	6-Deoxyglucose
Quinvosamine	2-Amino-2,6-dideoxyglucose
Rhamnitol (Rha-ol)	1-Deoxymannitol
Rhamnosamine (RhaN)	2-Amino-2,6-dideoxymannose
Rhamnose (Rha)	6-Deoxymannose
Ribose (Rib)	<i>ribo</i> -Pentose
Ribulose (Rul)	<i>erythro</i> -Pent-2-ulose
Sorbose (Sor)	<i>xylo</i> -Hex-2-ulose
Tagatose (Tag)	<i>lyxo</i> -Hex-2-ulose
Talose (Tal)	<i>talo</i> -Hexose
Tartaric acid	Erythraric/Threarric acid
Threose	<i>threo</i> -Tetrose
Xylose (Xyl)	<i>xylo</i> -Pentose
Xylulose (Xul)	<i>threo</i> -Pent-2-ulose

(b) common trivial names

Abequose (Abe)	3,6-Dideoxy-D-xylo-hexose
Amicetose	2,3,6-Trideoxy-D-erythro-hexose
Amylose	(1→4)-α-D-Glucopyranan
Apiose (Api)	3-C-(Hydroxymethyl)-glycero-tetrose
Arcanose	2,6-Dideoxy-3-C-methyl-3-O-methyl-xylo-hexose
Ascarylose	3,6-Dideoxy-L-arabino-hexose
Ascorbic acid	L-threo-Hex-2-enono-1,4-lactone
Boivinose	2,6-Dideoxy-D-gulose
Cellobiose	β-D-Glucopyranosyl-(1→4)-D-glucose
Cellotriose	β-D-Glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-D-glucose
Chacotriose	α-L-Rhamnopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→4)]-D-glucose
Chalcoses	4,6-Dideoxy-3-O-methyl-D-xylo-hexose
Cladinose	2,6-Dideoxy-3-C-methyl-3-O-methyl-L-ribo-hexose
Colitose	3,6-Dideoxy-L-xylo-hexose
Cymarose	6-Deoxy-3-O-methyl-ribo-hexose
2-Deoxyribose (dRib)	2-Deoxy-erythro-pentose
2-Deoxyglucose (2dGlc)	2-Deoxy-arabino-hexose
Diginose	2,6-Dideoxy-3-O-methyl-fyxo-hexose
Digitalose	6-Deoxy-3-O-methyl-D-galactose
Digitoxose	2,6-Dideoxy-D-ribo-hexose
Evalose	6-Deoxy-3-C-methyl-D-mannose
Evernitrose	2,3,6-Trideoxy-3-C-methyl-4-O-methyl-3-nitro-L-arabino-hexose
Gentianose	β-D-Fructofuranosyl β-D-glucopyranosyl-(1→6)-α-D-glucopyranoside
Gentiobiose	β-D-Glucopyranosyl-(1→6)-D-glucose
Hamamelose	2-C-(Hydroxymethyl)-D-ribose
Inulin	(2→1)-β-D-Fructofuranan
Isolevogluosenone	1,6-Anhydro-2,3-dideoxy-β-D-glycero-hex-2-enopyranos-4-ulose
Isomaltose	α-D-Glucopyranosyl-(1→6)-D-glucose
Isomaltotriose	α-D-Glucopyranosyl-(1→6)-α-D-glucopyranosyl-(1→6)-D-glucose
Isopanose	α-D-Glucopyranosyl-(1→4)-[α-D-glucopyranosyl-(1→6)]-D-glucose
Kojibiose	α-D-Glucopyranosyl-(1→2)-D-glucose
Lactose (Lac)	β-D-Galactopyranosyl-(1→4)-D-glucose
Lactosamine (LacN)	β-D-Galactopyranosyl-(1→4)-D-glucosamine
Lactosdiamine (LacdiN)	2-Amino-2-deoxy-β-D-galactopyranosyl-(1→4)-D-glucosamine
Laminarabiose	β-D-Glucopyranosyl-(1→3)-D-glucose
Levoglucofan	1,6-Anhydro-β-D-glucopyranose
Levoglucofenone	1,6-Anhydro-3,4-dideoxy-β-D-glycero-hex-3-enopyranos-2-ulose
Maltose	α-D-Glucopyranosyl-(1→4)-D-glucose
Manninotriose	α-D-Galactopyranosyl-(1→6)-α-D-galactopyranosyl-(1→6)-D-glucose
Melezitose	α-D-Glucopyranosyl-(1→3)-β-D-fructofuranosyl α-D-glucopyranoside
Melibiose	α-D-Galactopyranosyl-(1→6)-D-glucose
Muramic acid (Mur)	2-Amino-3-O-[(R)-1-carboxyethyl]-2-deoxy-D-glucose
Mycarose	2,6-Dideoxy-3-C-methyl-L-ribo-hexose
Mycinose	6-Deoxy-2,3-di-O-methyl-D-allose

Neuraminic acid (Neu)	5-Amino-3,5-dideoxy-D- <i>glycero</i> -D- <i>galacto</i> -non-2-ulosonic acid
Nigerose	α -D-Glucopyranosyl-(1 \rightarrow 3)-D-glucose
Nojirimycin	5-Amino-5-deoxy-D-glucopyranose
Noviose	6-Deoxy-5-C-methyl-4-O-methyl-L- <i>lyxo</i> -hexose
Oleandrose	2,6-Dideoxy-3-O-methyl-L- <i>arabino</i> -hexose
Panose	α -D-Glucopyranosyl-(1 \rightarrow 6)- α -D-glucopyranosyl-(1 \rightarrow 4)-D-glucose
Paratose	3,6-Dideoxy-D- <i>ribo</i> -hexose
Planteose	α -D-Galactopyranosyl-(1 \rightarrow 6)- β -D-fructofuranosyl α -D-glucopyranoside
Primeverose	β -D-Xylopyranosyl-(1 \rightarrow 6)-D-glucose
Raffinose	β -D-Fructofuranosyl α -D-galactopyranosyl-(1 \rightarrow 6)- α -D-glucopyranoside
Rhodinose	2,3,6-Trideoxy-L- <i>threo</i> -hexose
Rutinose	α -L-Rhamnopyranosyl-(1 \rightarrow 6)-D-glucose
Sarmentose	2,6-Dideoxy-3-O-methyl-D- <i>xylo</i> -hexose
Sedoheptulose	D- <i>altro</i> -Hept-2-ulose
Sedoheptulosan	2,7-Anhydro- β -D- <i>altro</i> -hept-2-ulopyranose
Solatriose	α -L-Rhamnopyranosyl-(1 \rightarrow 2)-[β -D-glucopyranosyl-(1 \rightarrow 3)]-D-galactose
Sophorose	β -D-Glucopyranosyl-(1 \rightarrow 2)-D-glucose
Stachyose	β -D-Fructofuranosyl α -D-galactopyranosyl-(1 \rightarrow 6)- α -D-galactopyranosyl-(1 \rightarrow 6)- α -D-glucopyranoside
Streptose	5-Deoxy-3-C-formyl-L- <i>lyxose</i>
Sucrose (saccharose)	β -D-Fructofuranosyl α -D-glucopyranoside
α , α -Trehalose	α -D-Glucopyranosyl α -D-glucopyranoside
Trehalosamine	2-Amino-2-deoxy- α -D-glucopyranosyl α -D-glucopyranoside
Turanose	α -D-Glucopyranosyl-(1 \rightarrow 3)-D-fructose
Tyvelose (Tyv)	3,6-Dideoxy-D- <i>arabino</i> -hexose
Umbelliferose	β -D-Fructofuranosyl α -D-galactopyranosyl-(1 \rightarrow 2)- α -D-galactopyranoside

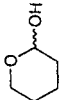

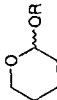
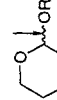
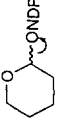
(c) trivial names formed by modification of non-standard monosaccharide parent names

Acosamine	3-Amino-2,3,6-trideoxy-L- <i>xylo</i> -hexose
Bacillosamine	2,4-Diamino-2,4,6-trideoxy-D-glucose
Daunosamine	3-Amino-2,3,6-trideoxy-L- <i>lyxo</i> -hexose
Desosamine	3,4,6-Trideoxy-3-dimethylamino-D- <i>xylo</i> -hexose
Forosamine	2,3,4,6-Tetradeoxy-4-dimethylamino-D- <i>erythro</i> -hexose
Garosamine	3-Deoxy-4-C-methyl-3-methylamino-L-arabinose
Kanosamine	3-Amino-3-deoxy-D-glucose
Kansosamine	4,6-Dideoxy-3-C-methyl-2-O-methyl-L-mannose
Mycaminose	3,6-Dideoxy-3-dimethylamino-D-glucose
Mycosamine	3-Amino-3,6-dideoxy-D-mannose
Perosamine	4-Amino-4,6-dideoxy-D-mannose
Pneumosamine	2-Amino-2,6-dideoxy-D-talose
Purpurosamine C	2,6-Diamino-2,3,4,6-tetradeoxy-D- <i>erythro</i> -hexose
Rhodosamine	2,3,6-Trideoxy-3-dimethylamino- <i>lyxo</i> -hexose

Glossary of Glycose-based Terms

Standard forms

[Common biochemical usage]

Class	Amino sugar ^d (usually as acetamido (N-acetyl) derivative)	Uronic acid ^b <i>Uronate</i>	Ulosonic acid <i>Ulosonate</i>	The sialic acid family ^b
Glycose 	Aminodeoxyglycose [Glycosamine]	Glycuronic acid <i>Glycuronate</i>	Glyculosonic acid <i>Glyculosonate</i> [Ketoglyconic acid]	Neuraminic acid Sialic acid
Glycosyl 	Aminodeoxyglycosyl [Glycosaminyl]	Glycosyluronic acid <i>Glycosyluronate</i> [Glycuronosyl]	Glyculosylonic acid <i>Glyculosylonate</i>	[Neuraminosyl] ^c [Sialosyl] ^c
Glycoside 	Aminodeoxyglycoside [Glycosaminide]	Glycosiduronic acid <i>Glycosiduronate</i> [Glycuronide]	Glyculosidonic acid <i>Glyculosidonate</i>	[Neuraminoside] [Sialoside]
Glycosidase (Glycoside hydrolase) 	Aminodeoxyglycosidase [Glycosaminidase]	Glycosiduronase [Glycuronidase]	Glyculosidonase	[Neuraminidase] [Sialidase]
Glycosyltransferase 	Aminodeoxyglycosyltransferase [Glycosaminyltransferase]	Glycosyluronatetransferase [Glycuronosyltransferase]	Glyculosylonattetransferase	[Neuraminosyltransferase] [Sialosyltransferase]

^dThe biochemical usage is widely established in the literature.^bThe biochemical usage implies the parents 'glycuronose', 'sialose', and 'neuraminose'.^c'Neuraminyl' and 'sialyl' have been used, but are likely to be interpreted as referring to acyl groups; the terms given are more consistent with the terms used for glycosides