Rules for Conformation Nomenclature for Five- and Six-membered Rings in Monosaccharides and their Derivatives

Following a text by J. C. P. Schwarz

The following rules have been approved by the British Carbohydrate Nomenclature Committee and by the U.S. Carbohydrate Nomenclature Committee. They will be submitted to IUPAC for international consideration.*

Rule 1. The approximate conformation of a five- or a six-membered ring in a carbohydrate may be indicated by an italic capital letter, designating the type of ring shape, and numerals, distinguishing between the variants of each shape (*e.g.* $^4C_1$).

Rule 2. The letter will be the appropriate one of the following:

Six-membered rings. *C* (for chair), *B* (for boat), *S* (for skew, *i.e.* the ' twist-boat ' midway between two boats in the cycle of flexible forms), *H* (for half-chair).

Five-membered rings. *E* (for envelope) and *T* (for twist *or* half-chair). The various shapes are illustrated in examples (1)—(16) and in the Figure.

Note. These representations are idealised, minor divergences being neglected.

Rule 3. The numerals will be the locants of the ring-atoms which lie outside a reference plane, defined for each conformation as below. (In furanoid and pyranoid rings, the ring oxygen, or other ring heteroatom, *e.g.* sulphur, will be denoted by its symbol, for example O or S). The locants of ring-atoms which lie on the side of the reference plane from which the numbering appears clockwise will be written as superscripts and will precede the letter; the locants of ring-atoms which lie on the other side of the reference plane will be written as subscripts and will follow the letter. [The numbering appears clockwise from the upper side of a furanoid or pyranoid Haworth formula written in the normal manner, but this may not be true for other rings, *e.g.* the benzylidene ring in example (13).]

* Other carbohydrate nomenclature topics under joint consideration are:

Oligosaccharides
Polysaccharides
Unsaturated monosaccharides
Branched-chain monosaccharides
Carbohydrate radicals
Carbohydrate derivatives of phosphorus acids
Monosaccharides in which there is unequal substitution at a carbon atom
Carbohydrate derivatives containing a heteroatom other than oxygen in the sugar ring
Carbohydrates with fused hetero-rings.

Further information or copies of the documents can be obtained from the Editor.

It is intended that after approval at national levels the rules will be submitted to IUPAC for consideration for the tentative forthcoming publication:

Carbohydrate Nomenclature—2 (Part 1 is IUPAC Information Bulletin—Appendices on Tentative Nomenclature, Symbols, Units, and Standards, number 7, 1970).

Rule 4. When the symbols are used for optically active species it must be made clear in the context whether the D- or L-form is referred to. Compounds that are *meso* will be regarded as belonging to the D-series for the purpose of defining the direction of numbering [examples (6) and (14)]. The conformation of a racemate will be indicated by the symbol appropriate for the D-enantiomer.

In a general discussion in which both D- and L-sugars are considered, symbols of the type $^{D}{}^4C_1$ could be used to define the conformation of an L-form by reference to the corresponding D-form.

Rule 5. In a ring other than a parent-sugar pyranoid or furanoid ring, the common ring carbon atom which bears the lowest number according to conventional carbohydrate nomenclature will be designated a1, the remaining ring atoms, including any heteroatoms, being numbered consecutively a2, a3, *etc.*, beginning with the relevant portion of the parent carbohydrate chain or ring [examples (12)—(16)], common to both rings. If there is more than one such ring, that ring associated with the lowest locant in the parent chain shall receive a-numbers, the next ring b-numbers, *etc.*

Rule 6. The reference plane for each ring shape will be chosen as follows (Note: some of the coplanarity relations implied in these rules are strictly true only for ideal rings with uniform bond lengths and angles):

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 (1)—(6) and (13)—(15)].

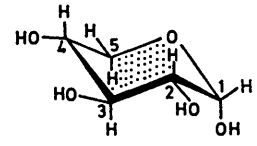
Possible conformations for aldopyranose rings: $^4C_1$ and $^1C_4$ (these correspond to Reeves's *C*1 and 1*C* conformations, respectively).

Boats. The reference plane is defined by the two ' sides ' of the boat [examples (7), (13), and (16)].

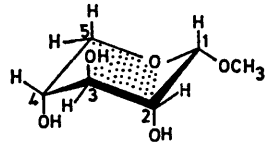
Possible conformations for aldopyranose rings: $^{1,4}B$, $B_{1,4}$, $^{2,5}B$, $B_{2,5}$, $^{O,3}B$, and $B_{O,3}$.

Skews. Each skew form has two potential reference planes, containing three adjacent atoms and the remaining non-adjacent atom. The reference plane is chosen so that the lowest-numbered carbon atom in the ring or the atom numbered next above it is exoplanar, in that order of preference [example (8) and Figure].

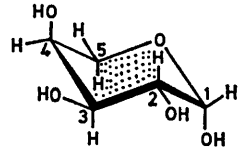
Possible conformations for aldopyranose rings: $^1S_3$, $^3S_1$, $^1S_5$, $^5S_1$, $^OS_2$, and ^2S_O.

(1)  $^4C_1$

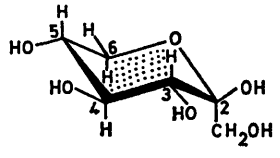
α-D-Xylopyranose

(2)  $^1C_4$

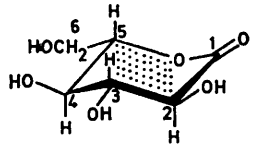
Methyl α-D-xylopyranoside

(3)  $^4C_1$

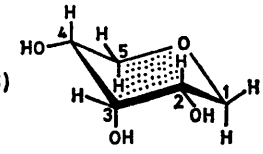
β-L-Arabinopyranose

(4)  $^5C_2$

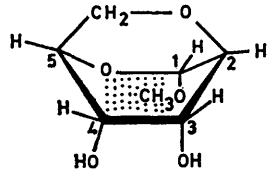
β-D-xylo-Hexulopyranose

(5)  $^1C_4$

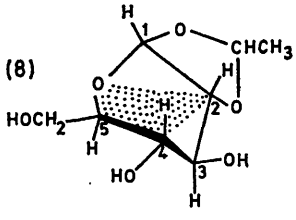
L-Glucono-1,5-lactone

(6)  $^4C_1$

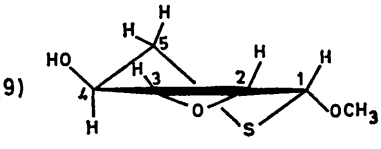
1,5-Anhydroribitol

(7)  $^{2,5}B$

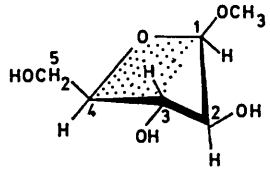
Methyl 2,6-anhydro-α-D-altropyranoside

(8)  $^1S_3$

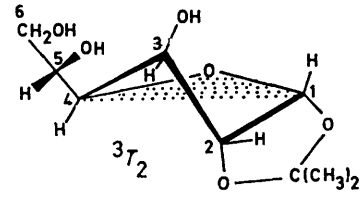
1,2-O-ethylidene-α-D-glucopyranose

(9)  $^5H_0$

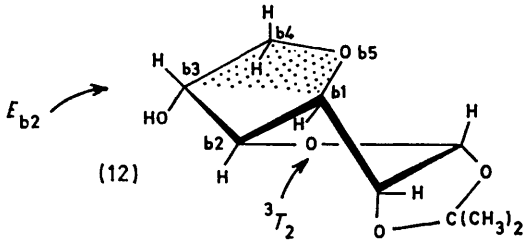
Methyl 2,3-anhydro-5-thio-β-L-lyxopyranoside

(10) 

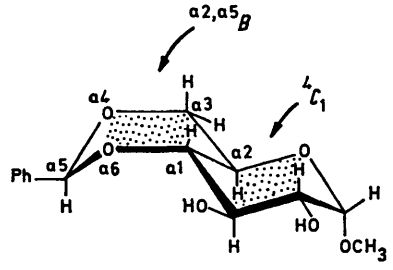
Methyl β-D-arabinofuranoside

(11) 

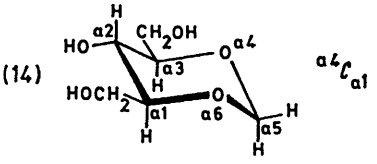
1,2-O-isopropylidene-β-L-idofuranose



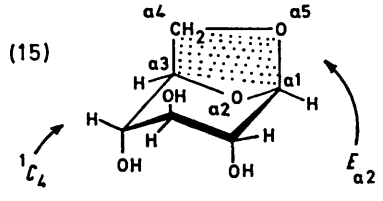
3,6-anhydro-1,2-O-isopropylidene-α-D-glucofuranose

(13) 

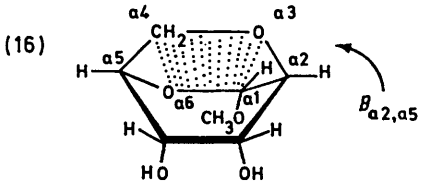
Methyl 4,6-O-benzylidene-α-D-glucopyranoside
(with the unusual configuration at the benzylidene carbon atom)

(14) 

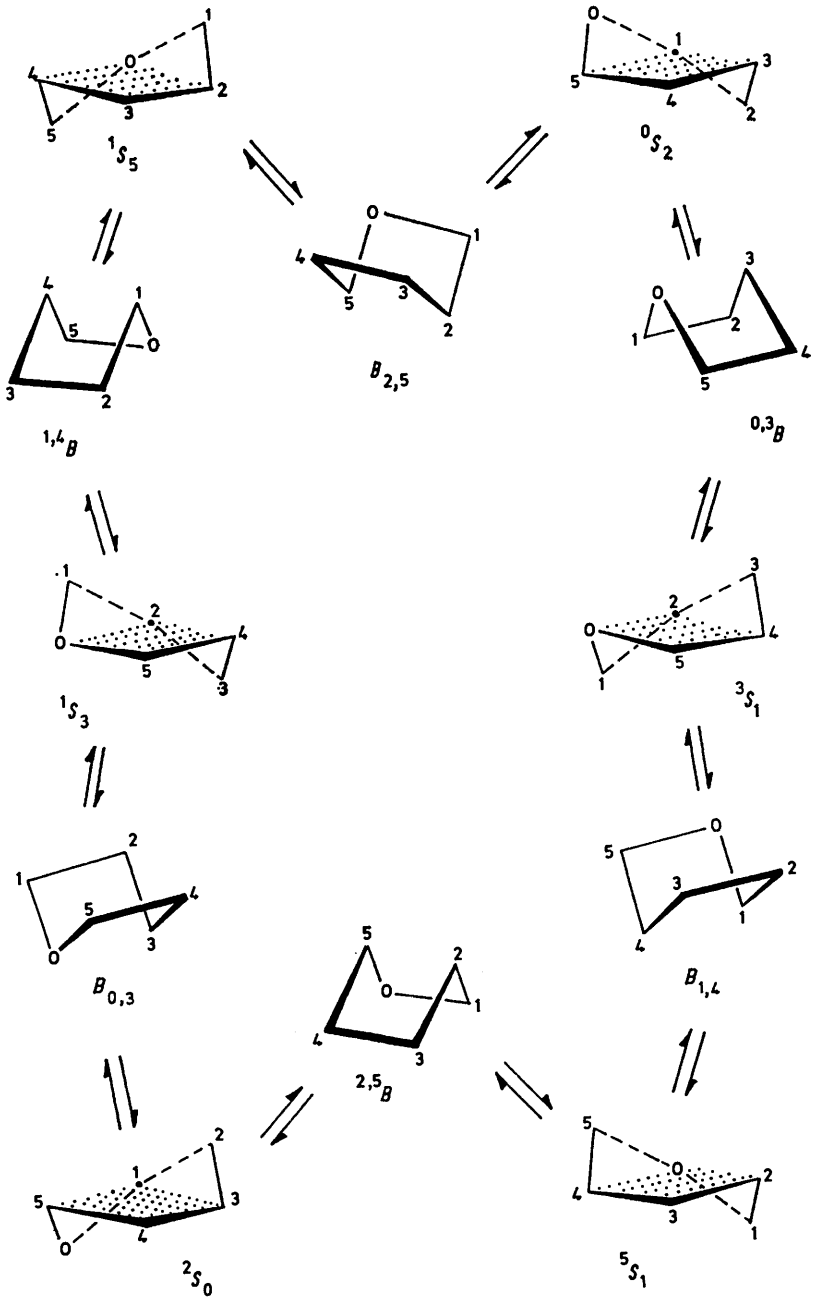
2,4-O-methyleneribitol

(15) 

1,6-anhydro-β-D-glucopyranose

(16) 

Methyl 2,6-anhydro-α-D-altropyranoside



The flexible boat skew cycle for aldopyranoses

(These symbols are related to those for the boat conformations; for example $^1S_5$ lies between $^{1,4}B$ and $B_{2,5}$ in the cycle of flexible forms shown in the Figure.)

Half-chairs. The reference plane is defined by the four adjacent coplanar atoms [example (9)].

Possible conformations for aldopyranose rings: $^OH_1$, ^1H_O, $^1H_2$, $^2H_1$, $^2H_3$, $^3H_2$, $^3H_4$, $^4H_3$, $^4H_5$, $^5H_4$, ^5H_O, and $^OH_5$.

Five-membered rings

Envelopes. The reference plane is defined by the four adjacent coplanar atoms [examples (10), (12), and (15)].

Possible conformations for aldofuranose rings: ^1E, E_1, ^2E, E_2, ^3E, E_3, ^4E, E_4, ^OE, and E_O.

Twists. The reference plane is defined by three adjacent ring-atoms, chosen so that the exoplanar atoms lie on opposite sides of the plane [examples (11) and (12)].

Possible conformations for aldofuranose rings: $^OT_1$, ^1T_O, $^1T_2$, $^2T_1$, $^2T_3$, $^3T_2$, $^3T_4$, $^4T_3$, ^4T_O, and $^OT_4$.